Lattice QCD calculations of NN interactions and prospects for parity violating matrix elements

INT Workshop 19R-76
Hadronic Parity Nonconservation II
24-27 January, 2022

André Walker-Loud

BERKELEY LAB

Outline

- ❑ Role of lattice QCD in understanding hadronic parity violation

- ❑ Anatomy of lattice QCD calculations
  - ❑ "regular" lattice QCD calculations
  - ❑ Hadronic parity violating matrix elements
  - ❑ Challenges in these calculations

- ❑ Status of lattice QCD calculations of two-nucleon systems
  - ❑ NN Controversy and its most-likely resolution
  - ❑ Momentum space to momentum space NN calculations in some detail
  - ❑ Prospects for new methods for calculating nucleon and NN matrix elements

- ❑ Promising prospects for controlled lattice QCD calculations of hadronic parity violating matrix elements

Role of lattice QCD in understanding hadronic PV

- Lattice QCD offers the promise of first principles theoretical predictions for nuclear physics
  - The only inputs for lattice QCD are the gauge coupling (β), the quark masses (m_u, m_d, m_s, [m_c]), the electromagnetic coupling, α_{fs}, the Fermi weak constant G_F
    Everything else is a prediction

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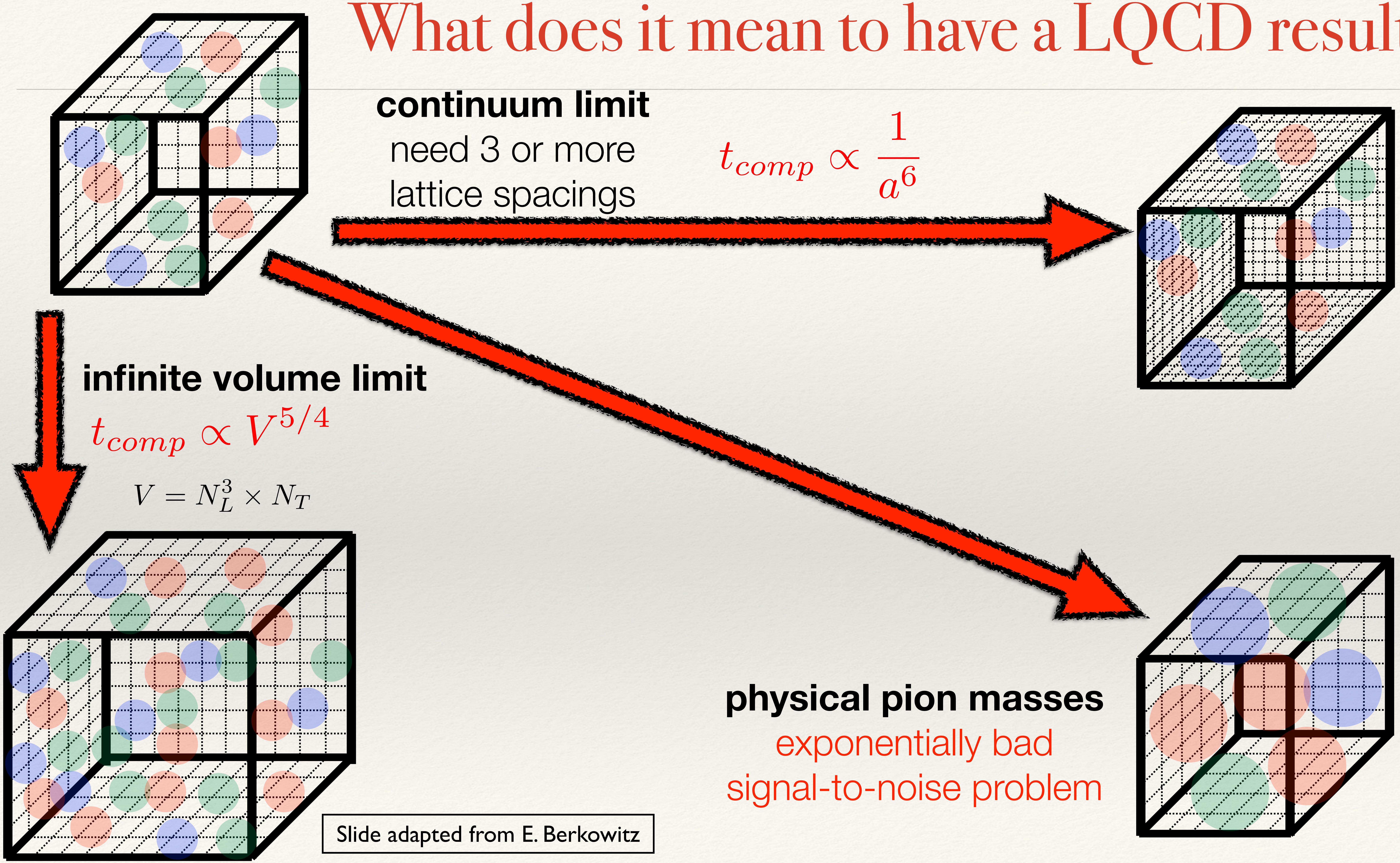
- So where are all the great results?

- Well, these calculations are difficult… (excuses, excuses, excuses…)

- Recently, there have been exciting "breakthrough" progress in NN calculations that makes me optimistic we will see meaningful progress towards PV in the next few years

- Once we convince ourselves, and the community, that we have our systematics under control
  - LQCD can provide results that compliment the experimental measurements,
  - Can be treated as additional, simple systems used to constrain the PV LECs
  - The LQCD results can be analyzed in concert with experimental data

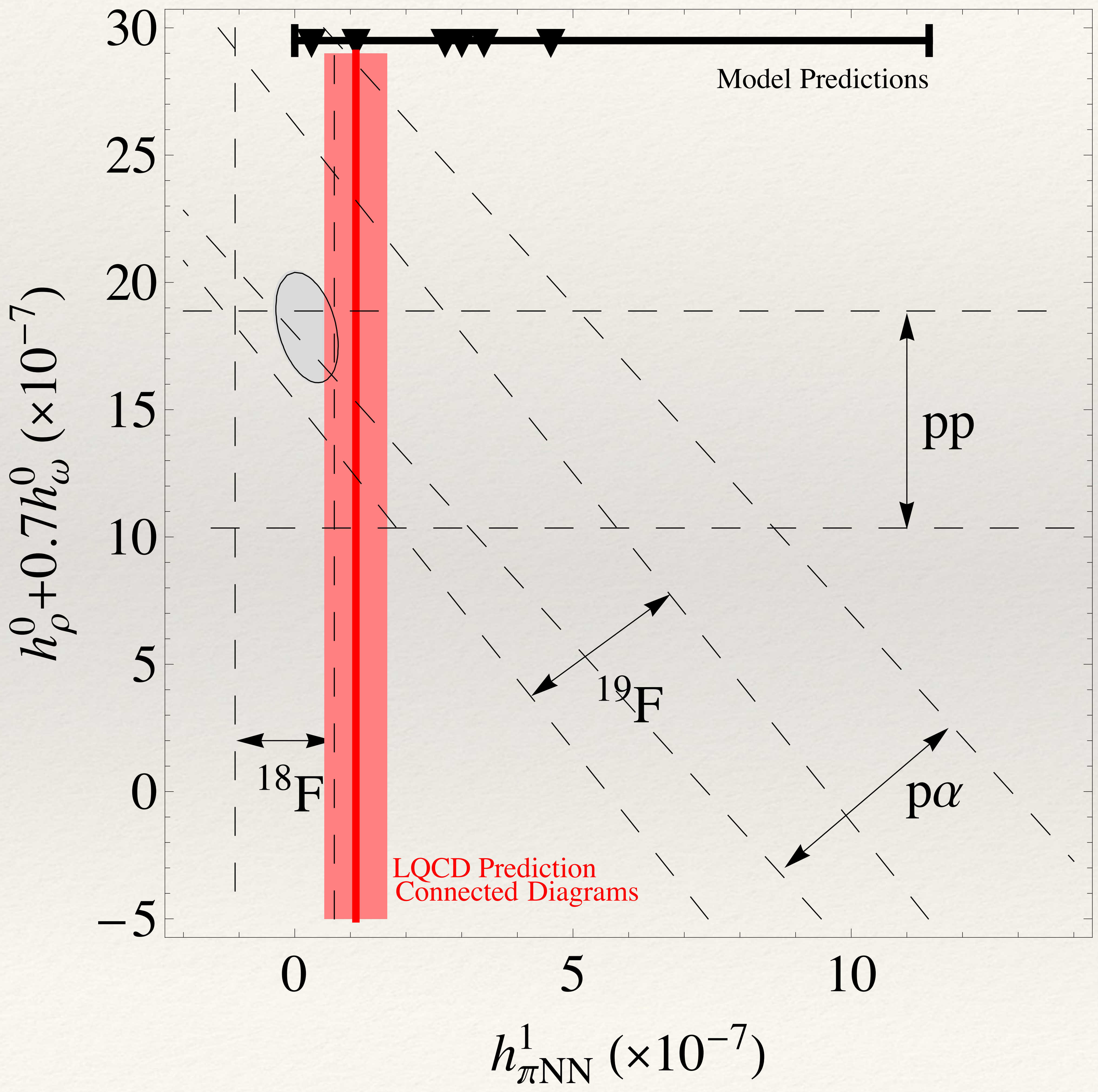
What does it mean to have a LQCD result?



Slide adapted from E. Berkowitz

What does it mean to have a LQCD result?

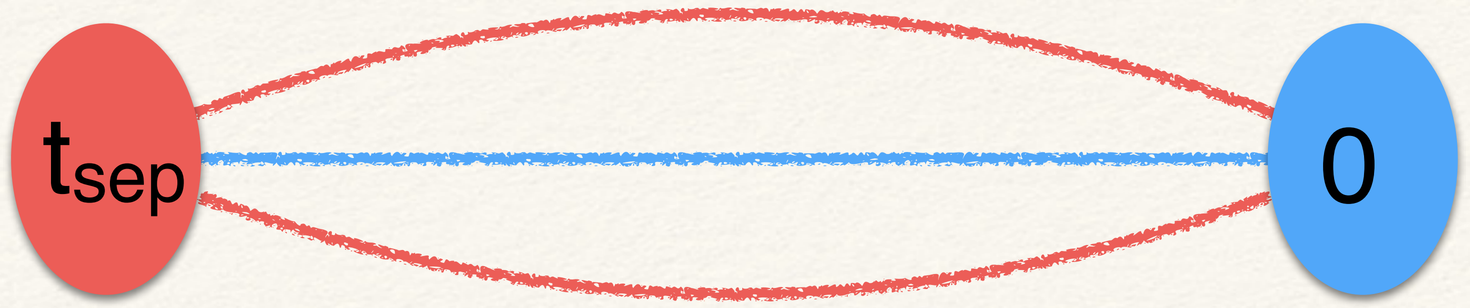
Wasem, PRC 85 (2012) [1108.1151] (tour de force - no new result since then)



First LQCD calculation	✓
Numerical result	✓
use of good operator basis	✗
control over renormalization	✗
control over finite-V to inf-V	✗
control over disconnected diagram	✗
control of excited states	✗
control over chiral extrapolation	✗

- This result has an unquantified systematic uncertainty
- it is possible they all conspire to cancel and agree with the NPDGamma result
- This needs to be validated/cross checked

LQCD: 2 point functions



$$C(t, \mathbf{p}=0) = \sum_{\mathbf{x}} \langle \Omega | N(t, \mathbf{x}) N^\dagger(0, \mathbf{0}) | \Omega \rangle$$

$$= A_0 e^{-E_0 t} \left(1 + \sum_{n>0} r_n e^{-\Delta_{n0} t} \right)$$

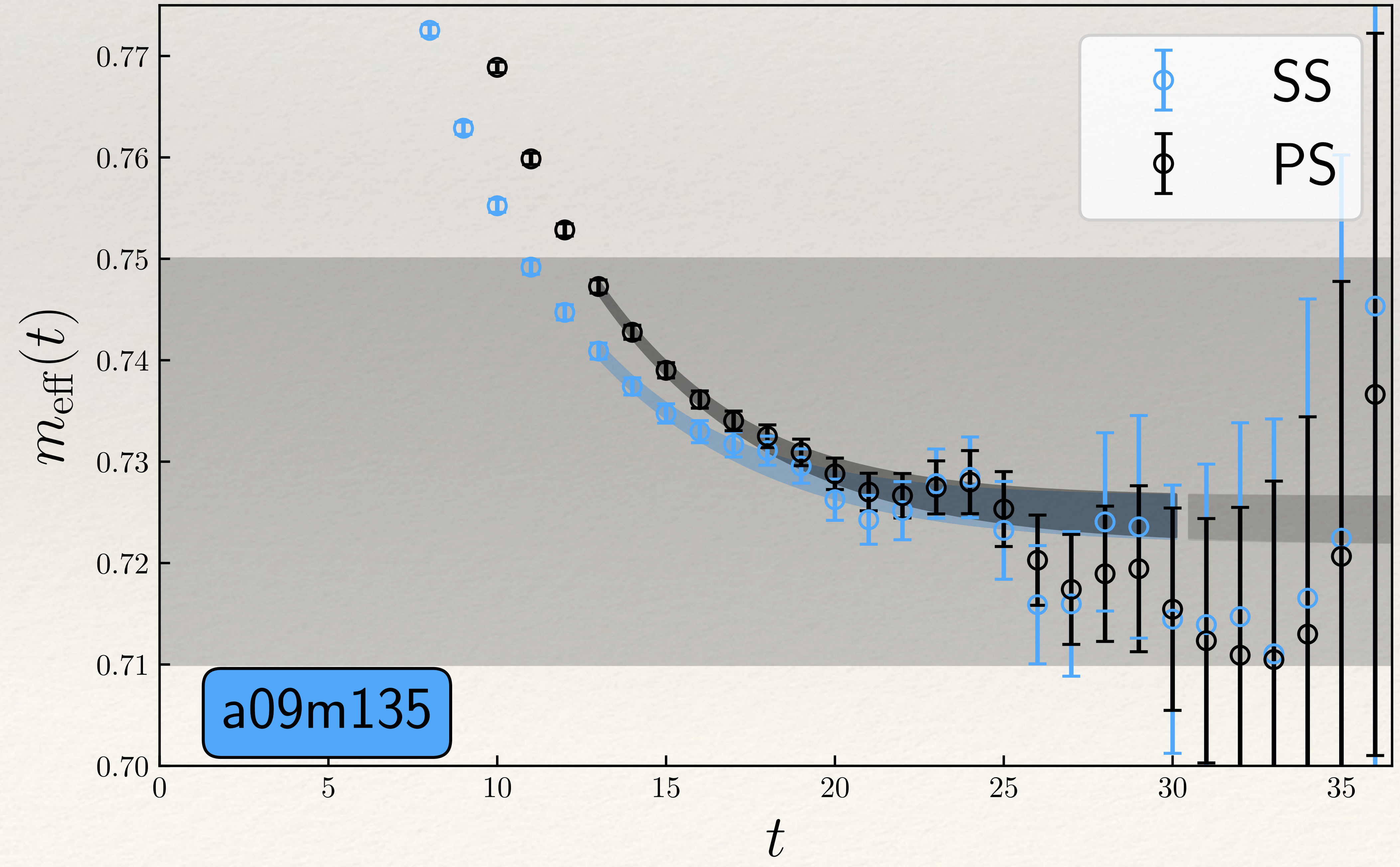
$$\Delta_{n0} = E_n - E_0$$

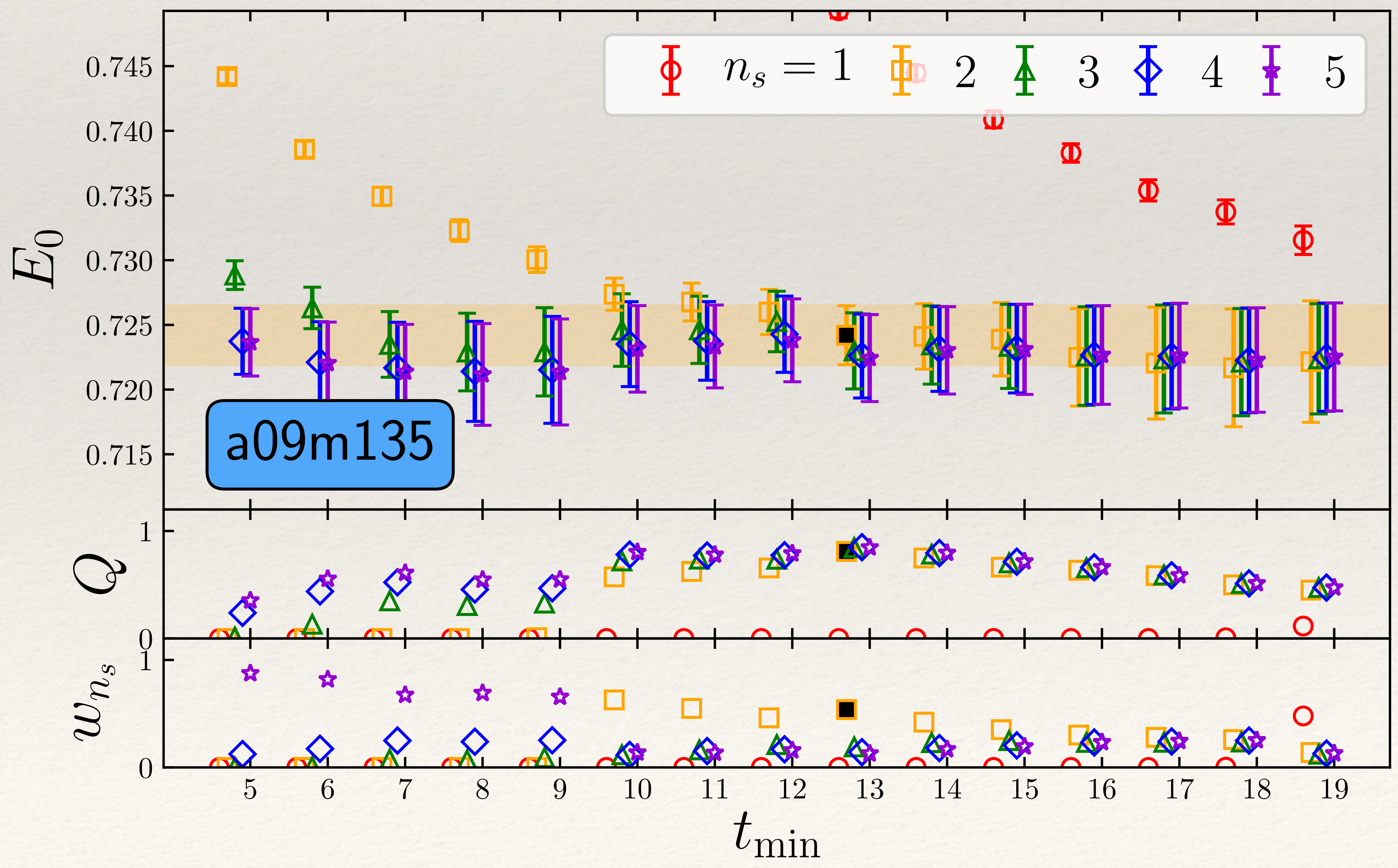
$$m_{\text{eff}}(t) = \ln \left(\frac{C(t)}{C(t+1)} \right) \underbrace{\longrightarrow}_{\text{large } t} E_0 + \sum_{n>0} r_n \left(e^{-\Delta_{n0} t} - e^{-\Delta_{n0} t + 1} \right)$$

NOTE: if the creation operator is conjugate to the annihilation operator

$$r_n \geq 0$$

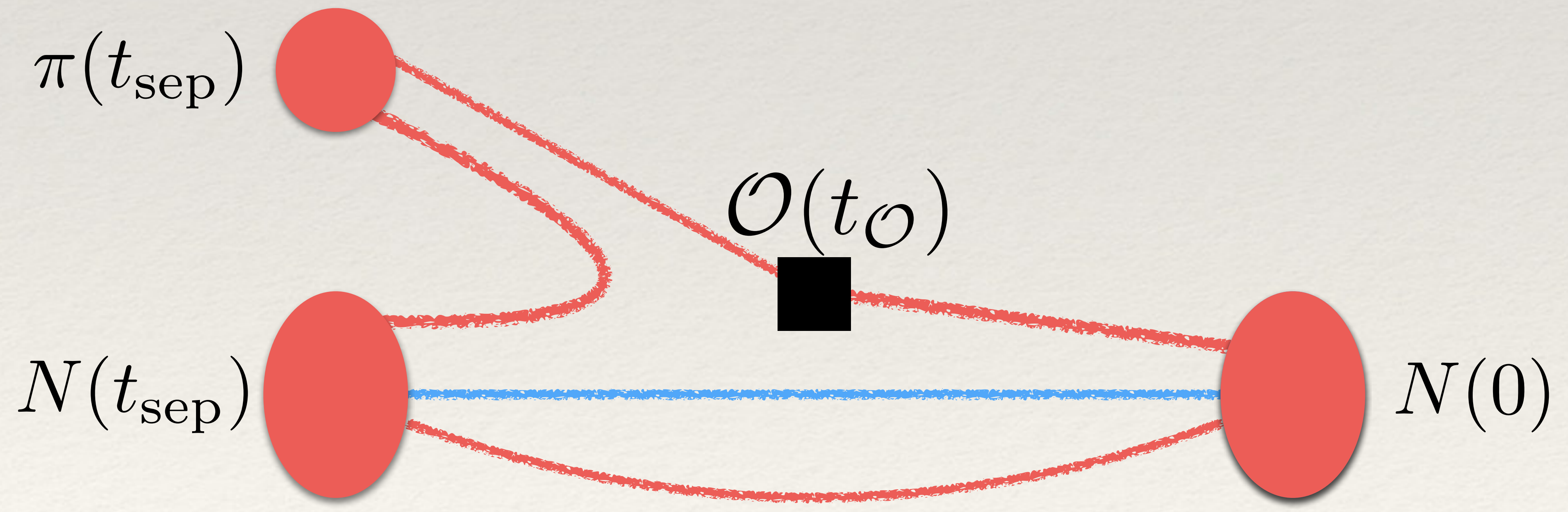
but… signal-to-noise



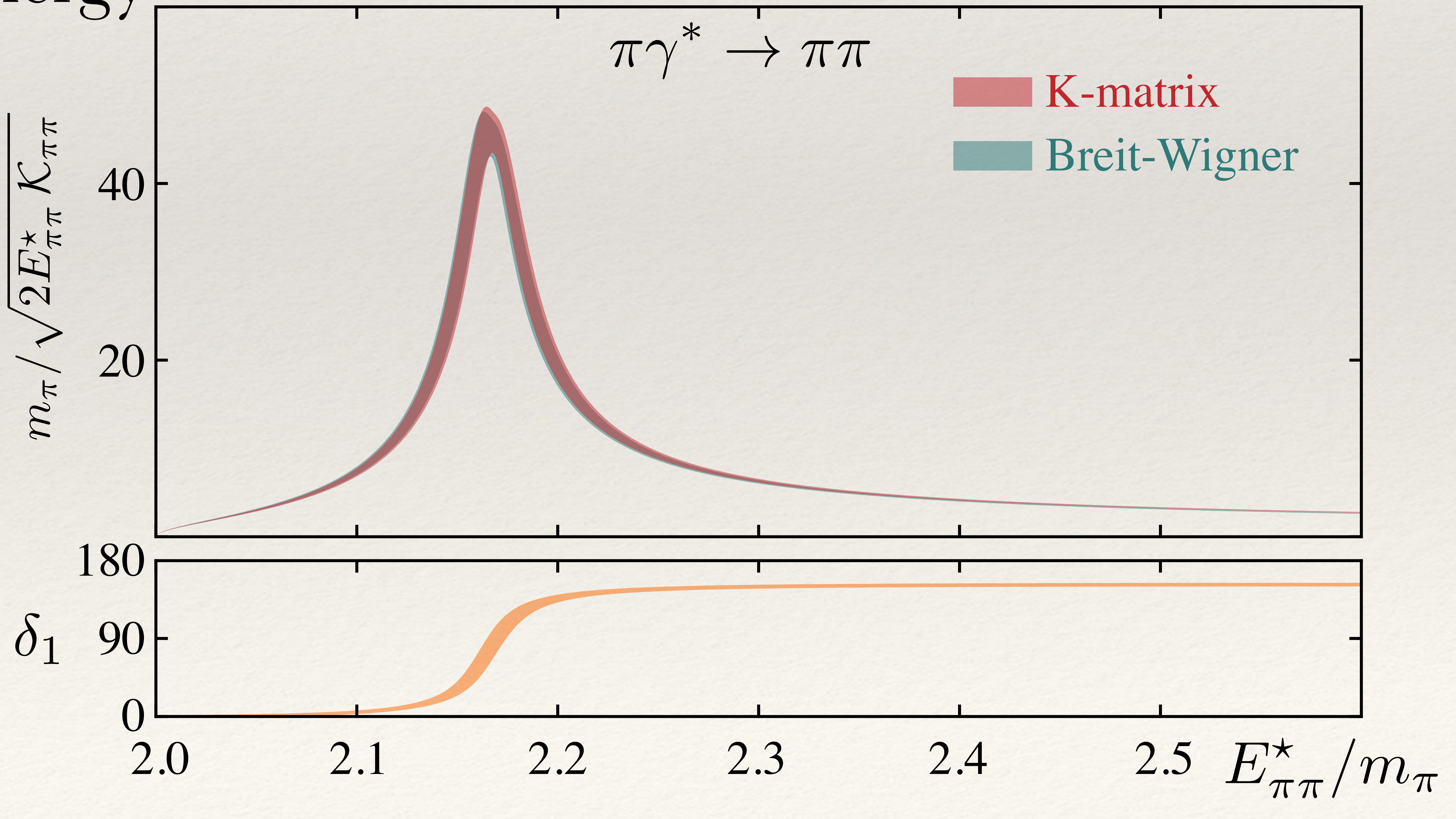


LQCD: 2 point functions

- Parity violating matrix elements involve multi-hadrons in the initial and/or final state
  - 2-hadron spectroscopy brings additional, substantial challenges (sources of systematic uncertainty)
    - The relative stochastic noise is worse
    - The physics of interest resides in the relatively small interaction energy
  - Isolating the ground state is exponentially more challenging
  - Critical to know the multi-hadron interaction energy
    FV ME → Inf. V ME depends on phase shift
    can be O(100% or more) effect



Briceno et al, PRD 93 (2016) [1604.03550]



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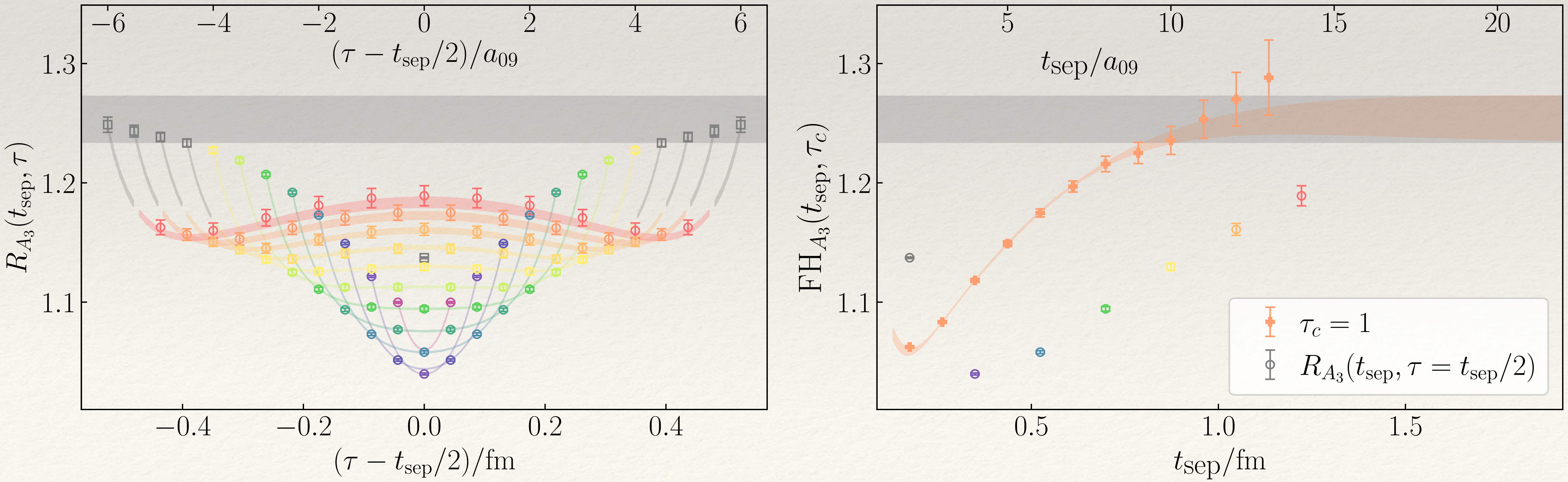
    - (or we are stuck with significant excited state contamination)



He et al (CalLat) 2104.05226

calculation of gA focussing on understanding excited state contamination

Mpi~310 MeV

Physical pion mass:
more noise
more ex. state contamination

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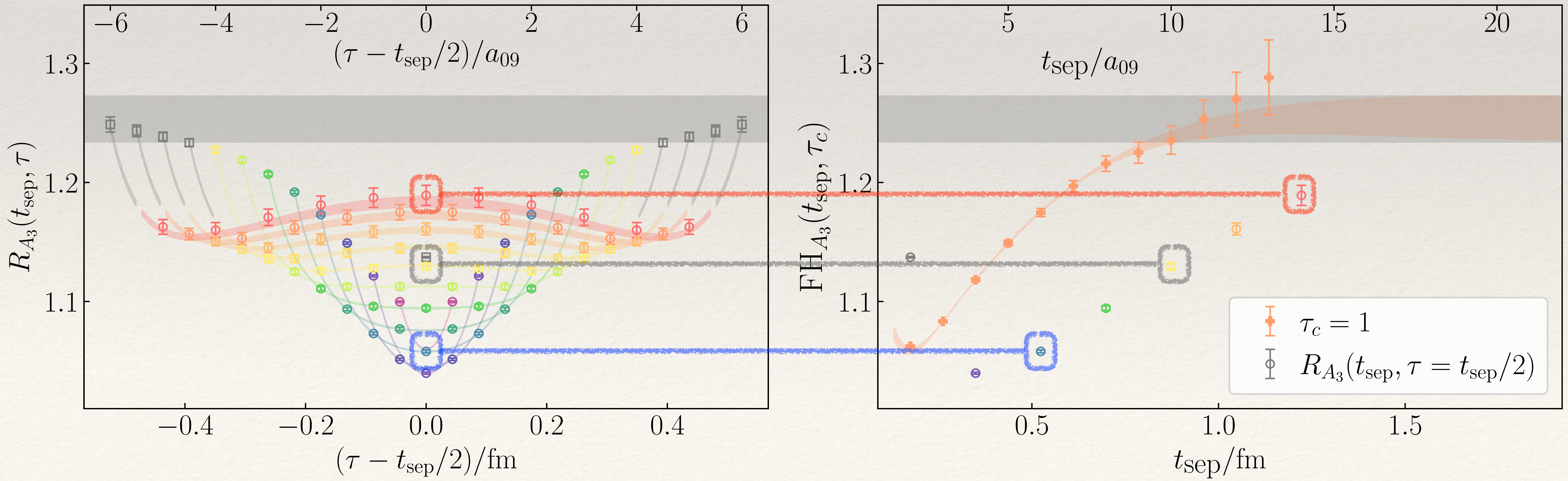

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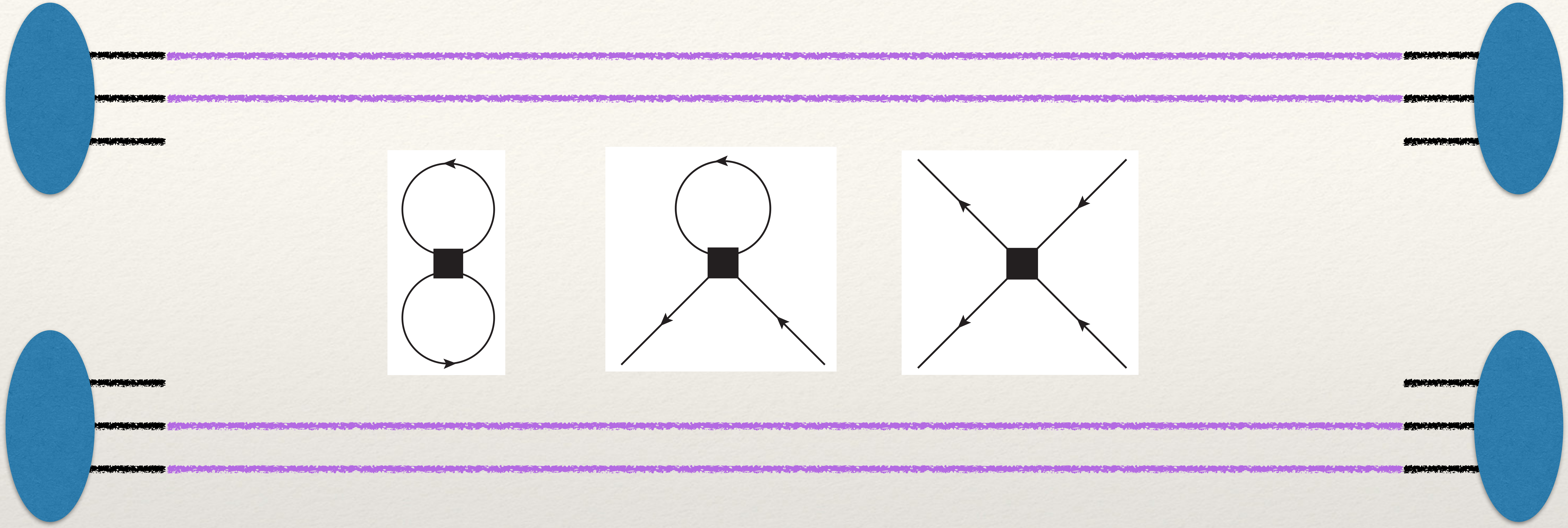
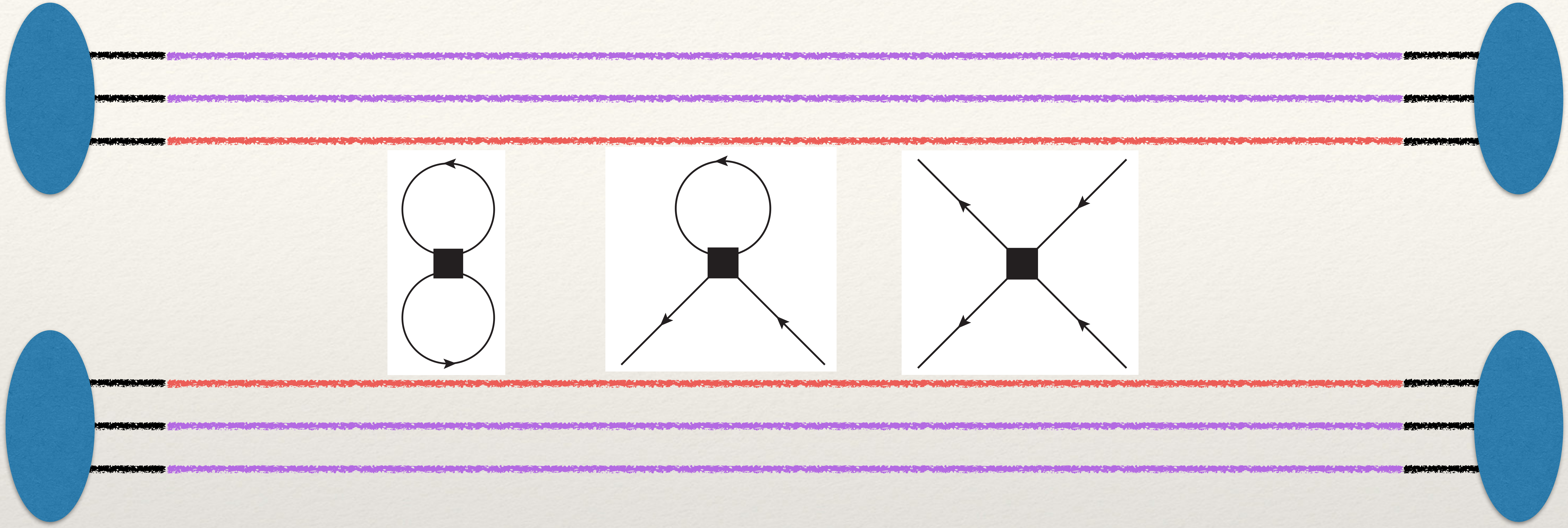
LQCD: NN matrix elements

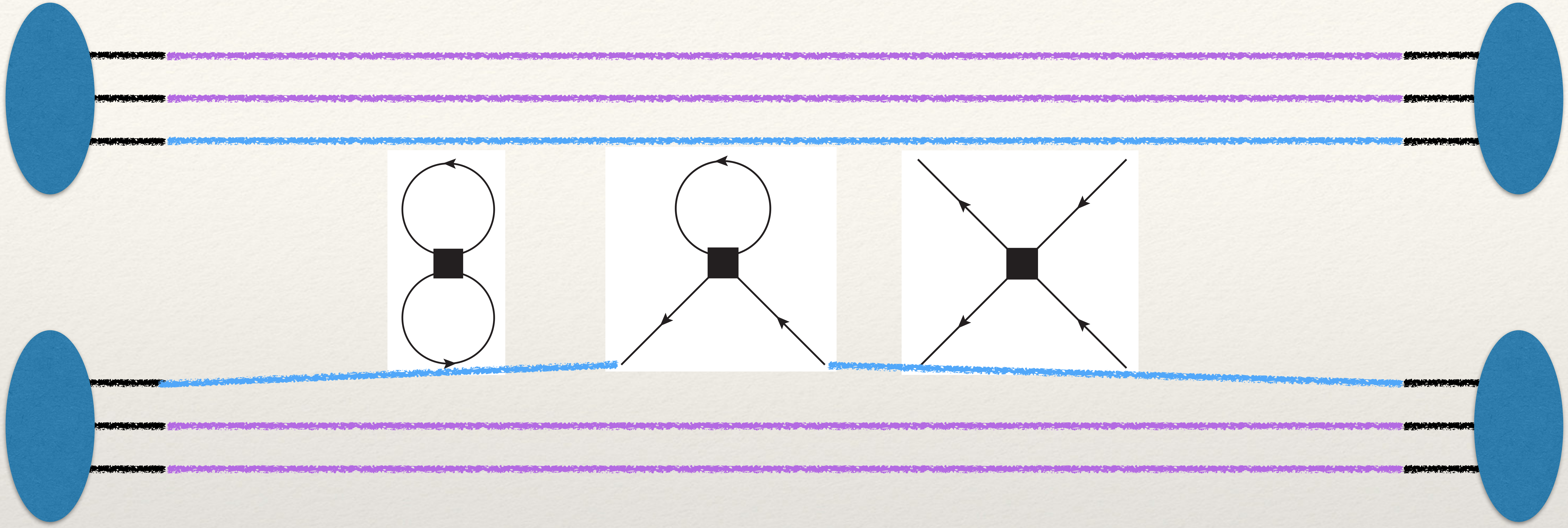


LQCD: NN matrix elements



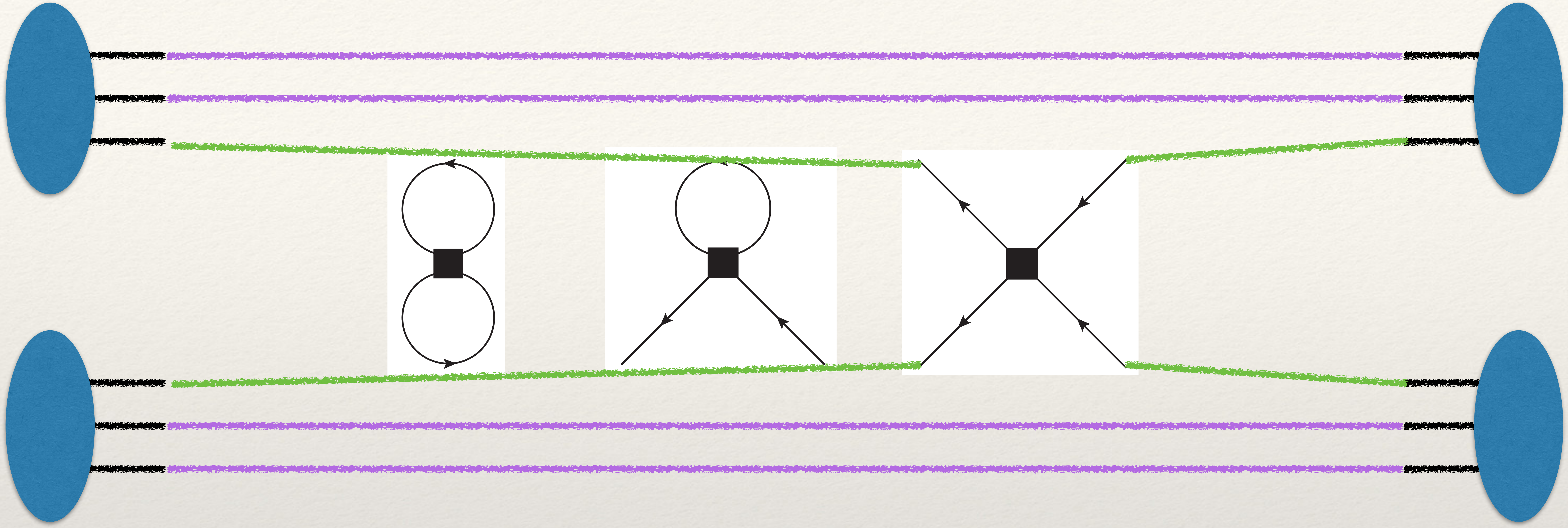
ΔI=0

LQCD: NN matrix elements



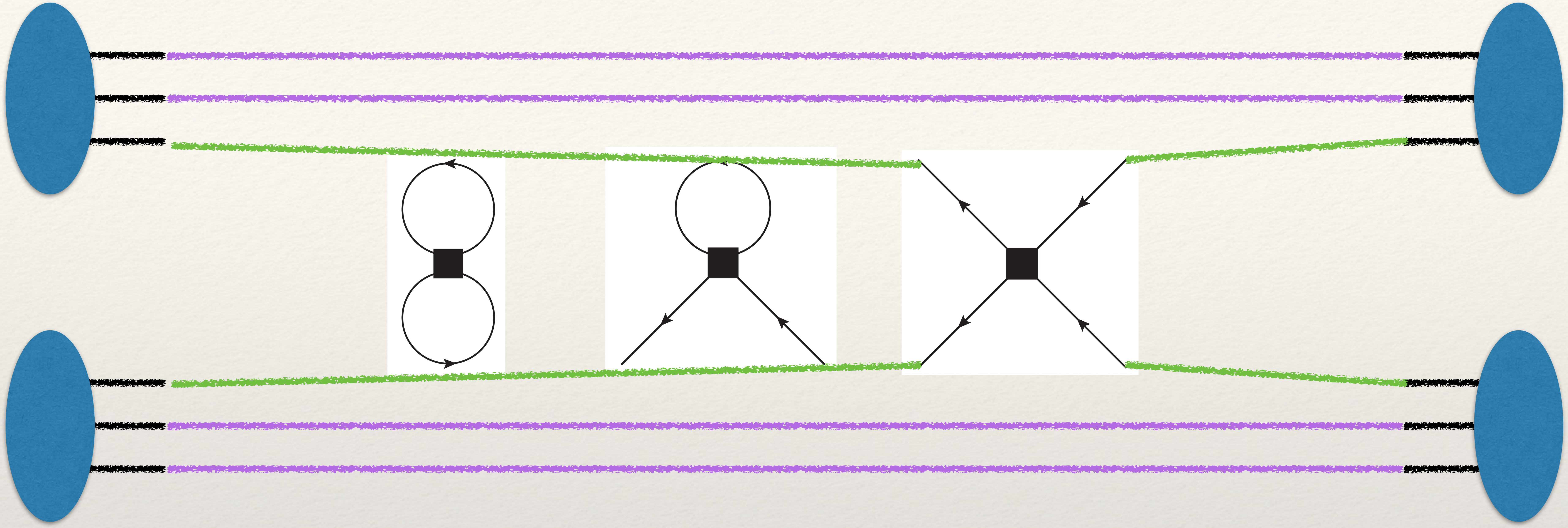
ΔI=0,1

LQCD: NN matrix elements



ΔI=0,1,2

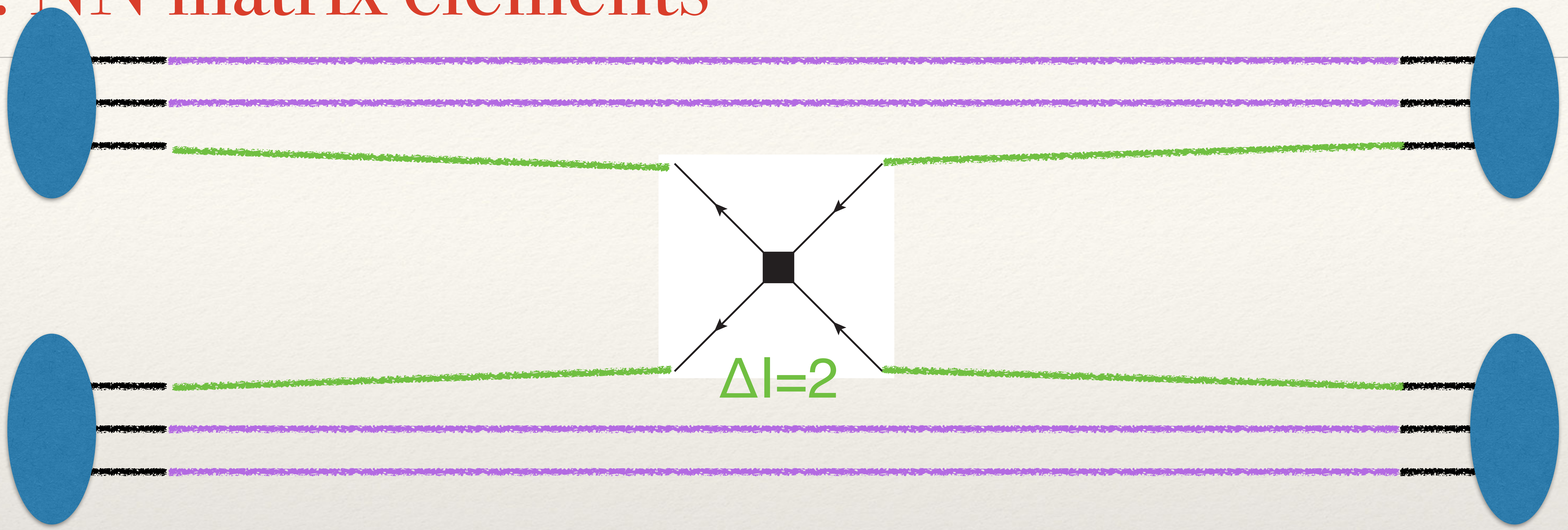
LQCD: NN matrix elements



ΔI=0,1,2

- The “disconnected” quark loops are numerically more expensive, and stochastically noisier
- The non-perturbative renormalization becomes more challenging also (eg. ΔI=0 mixes with the vacuum - power-divergent mixing :O)

LQCD: NN matrix elements



$NN(t, \mathbf{x})$ $\mathcal{O}(t_{\mathcal{O}}, \mathbf{z})$ $N^\dagger N^\dagger(0, \mathbf{0})$

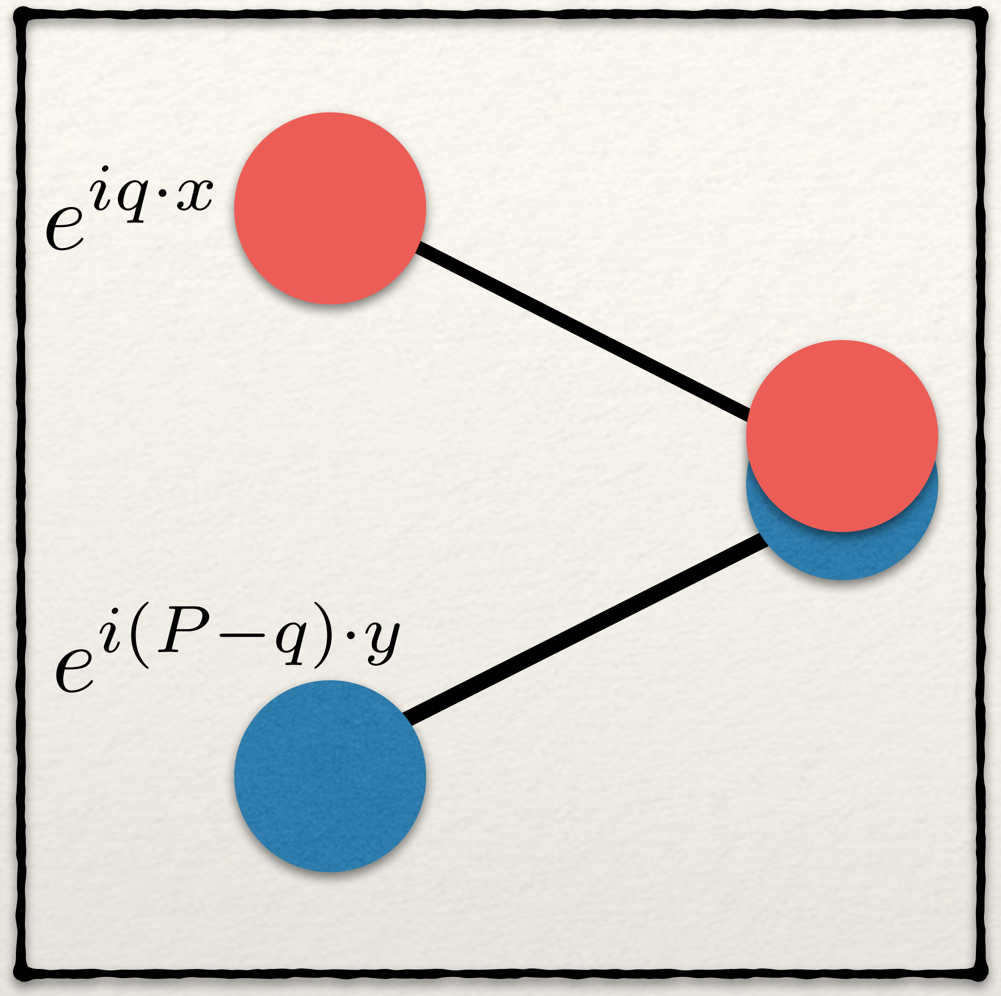
- To project the operator, *O*, onto definite momentum, and to project the final NN state onto definite momentum, we need all-to-all propagators (expensive): $\sum_{\mathbf{x}}, \sum_{\mathbf{z}}$

- Not possible with (old) standard NN calculations with local creation operators and momentum space annihilation operators

LQCD: NN matrix elements

- We started the $\Delta I=2$, NN calculation in 2015 Kurth et al., 1511.02260
- Ultimately, we decided that the growing concern regarding the NN bound-state controversy, combined with the challenge of performing the 4-quark matrix element calculation, were too severe to proceed
- So we went back to basics to improve our NN calculations before trying to tackle the parity violating matrix element calculations

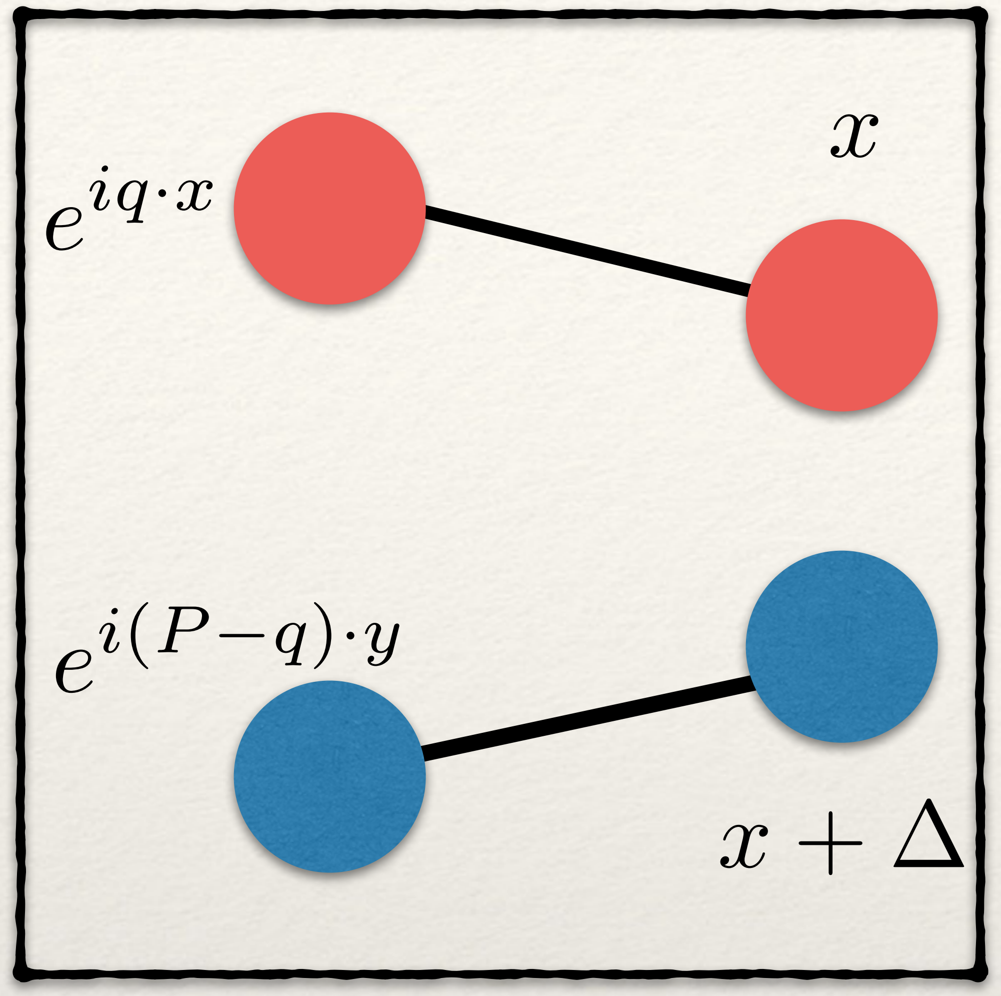
Two-nucleon controversy/discrepancy



Deep Bound States

NPLQCD
Yamazaki et al
CalLat

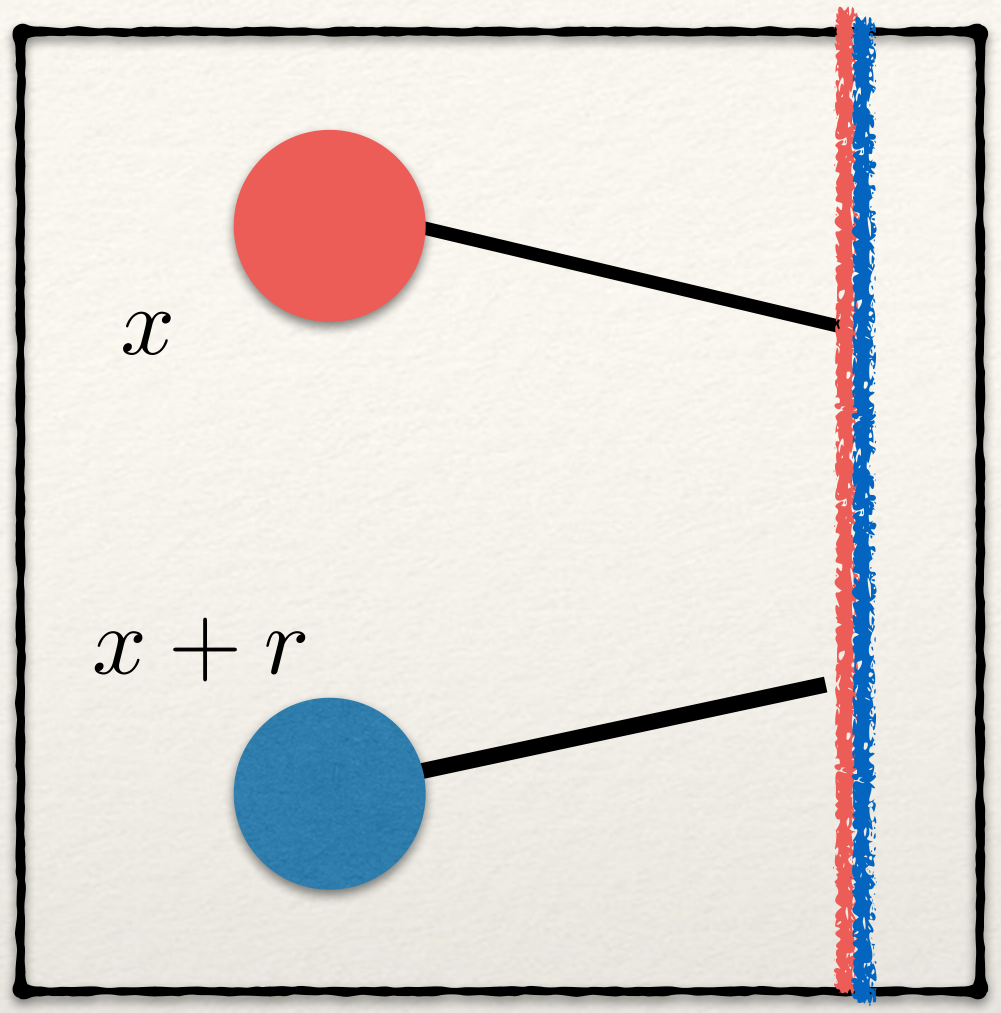
Compact, hexa-quark creation operator



Shallow/no Bound State

CalLat

“diffuse” non-local creation operator

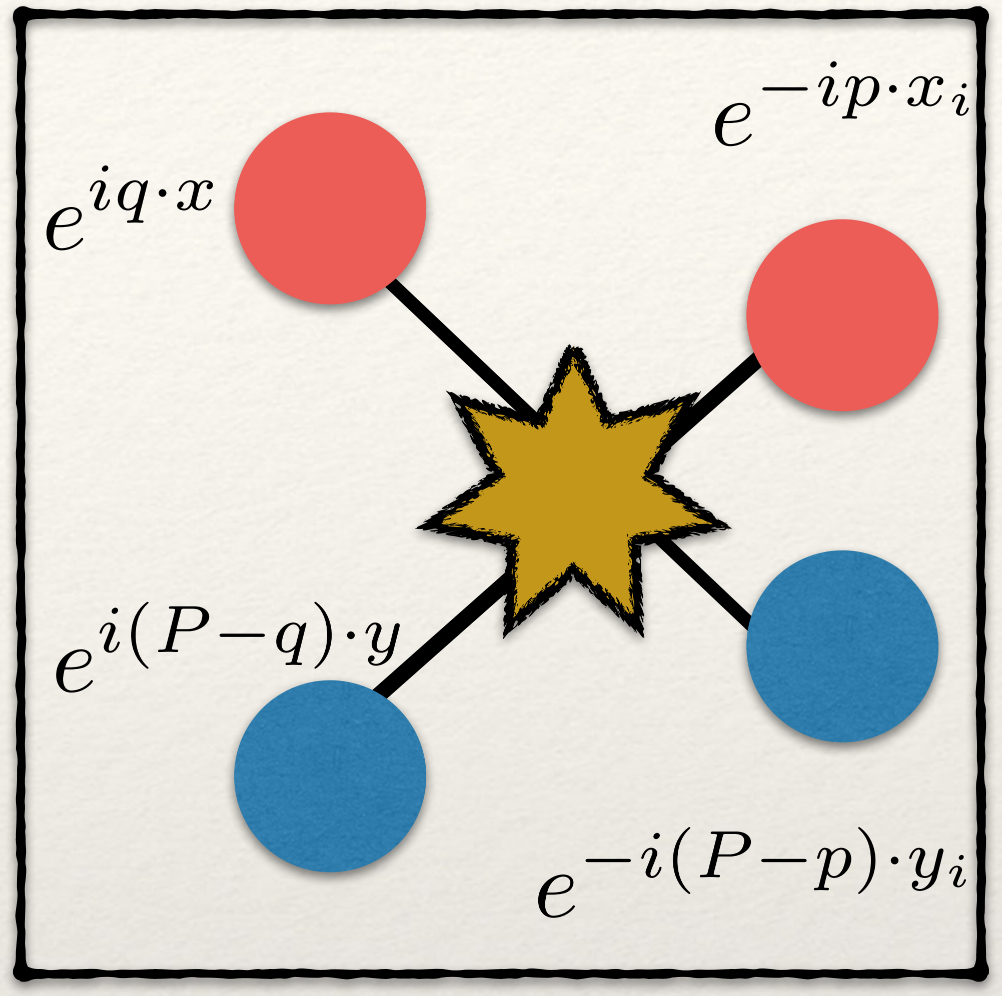


no Bound State

HAL QCD

$V(r) \to \delta(p)$

“diffuse” wall-source creation operator



no Bound State

Mainz, sLapHnn

(NPLQCD 2021)

“diffuse” momentum-space creation operator

- The spectrum does not depend upon the creation/annihilation operators
  - at least one method must be wrong

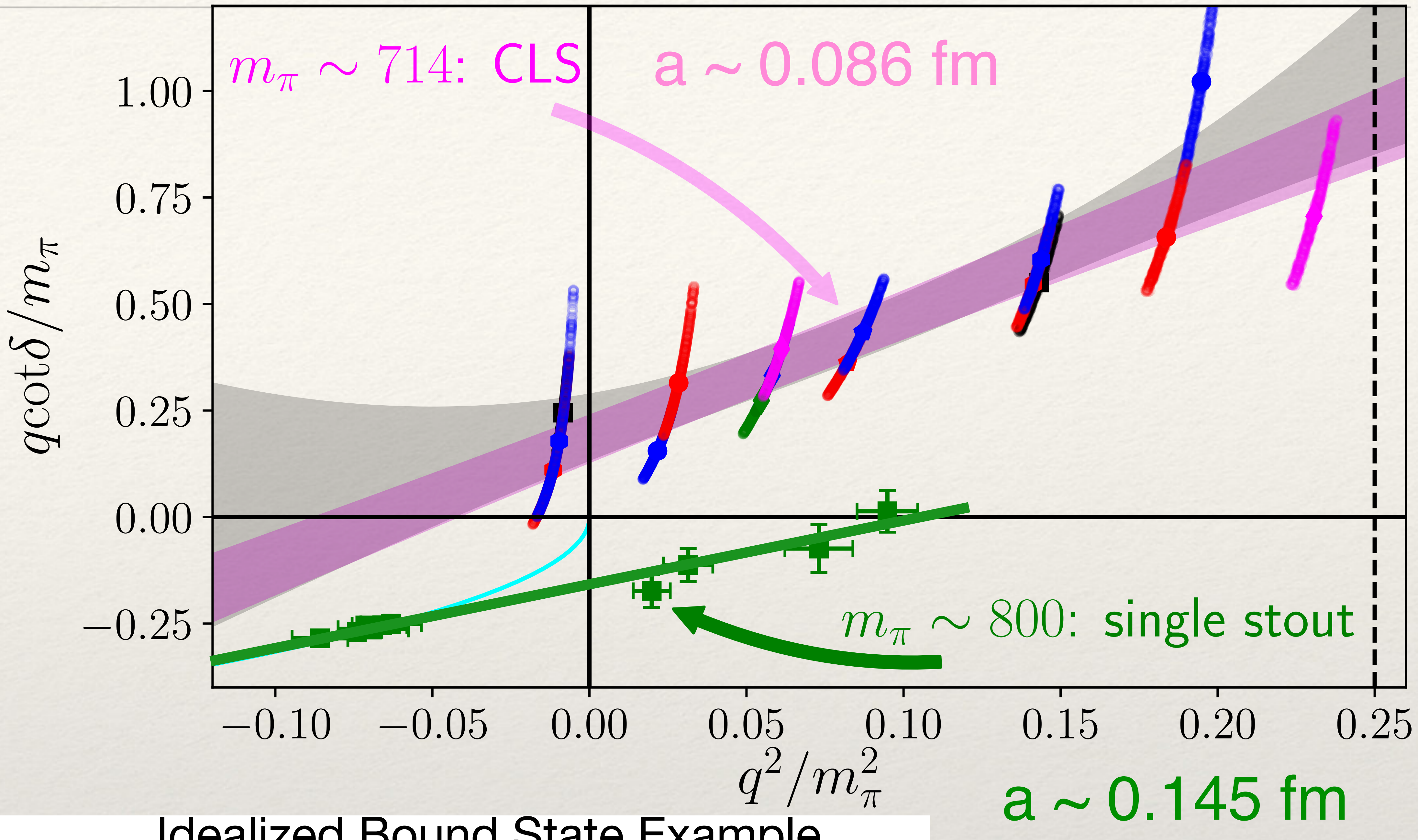
Comparing variational to older NPLQCD

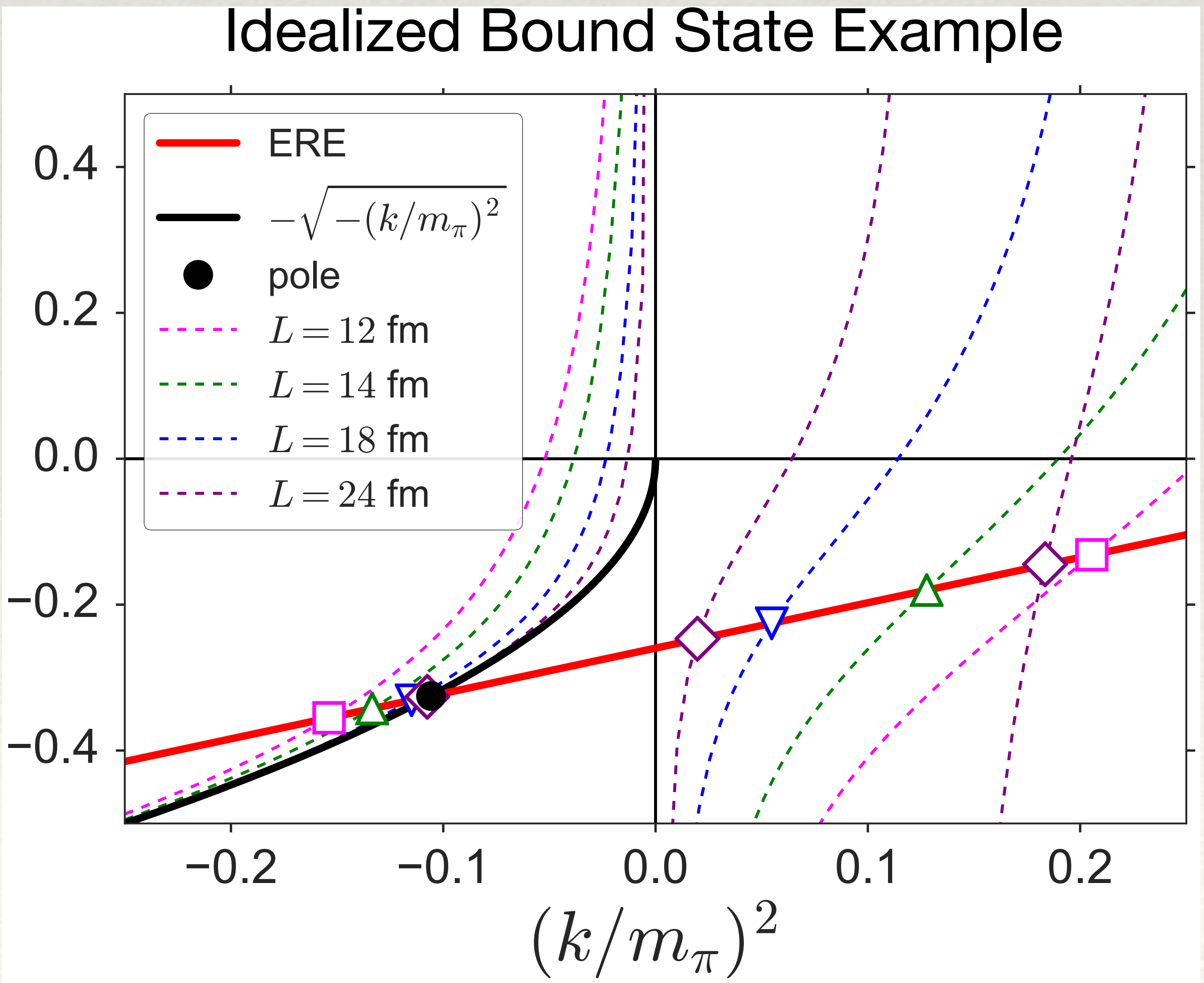
- Our results are in clear contradiction to NPLQCD at a similar pion mass
  - NPLQCD results were generated with local hexaquark creation operators
    - could this local operator couple more strongly to a deep bound state?
    - If so - our entire spectrum would have to shift down (similarly, NPLQCD would have to shift up)
  - Could it be a discretization effect?
    - Community expectation that discretization effects will not qualitatively alter the nature of bound or not bound

But - will return to this point

I will comment - without showing details (some backup slides) - there is a preponderance of evidence that, the local creation operators (NPLQCD, CalLat 2015, Yamazaki et al), lead to a misidentification of the spectrum

- unquantified systematic uncertainty in phase shifts
- unquantified systematic uncertainty in all matrix elements





HAL QCD
PRD 96 (2017)
[1703.07210]

NN with sLapH

arXiv:2009.11825

Mpi~714 MeV

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covering nuclear physics

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Two-nucleon S-wave interactions at the SU(3) flavor-symmetric point with $m_{ud} \approx m_s^{\text{phys}}$: A first lattice QCD calculation with the stochastic Laplacian Heaviside method

Ben Hörz, Dean Howarth, Enrico Rinaldi, Andrew Hanlon, Chia Cheng Chang (張家丞), Christopher Körber, Evan Berkowitz, John Bulava, M. A. Clark, Wayne Tai Lee, Colin Morningstar, Amy Nicholson, Pavlos Vranas, and André Walker-Loud

Phys. Rev. C **103**, 014003 – Published 19 January 2021

for lack of a better name - sLapHnn Collaboration
(stochastic Laplacian Heaviside NN)

NN with sLapH

arXiv:2009.11825

Mpi~714 MeV

- "Traditional" method: local creation momentum annihilation
  $$C_{NN}(t,\mathbf{p}+\mathbf{q}) = \sum_{\mathbf{x}}\sum_{\mathbf{y}} e^{i\mathbf{p}\cdot\mathbf{x}} e^{i\mathbf{q}\cdot\mathbf{y}} \langle 0|N(t,\mathbf{x})N(t,\mathbf{y})N^\dagger(0,\mathbf{0})N^\dagger(0,\mathbf{0})|0\rangle$$
- sLapH (and distillation) momentum creation momentum annihilation positive definite correlator ($r_n \geq 0$) Diagonalize correlator with GEVP
  $$C_{ij}^{NN}(t,\mathbf{p_f},\mathbf{q_f},\mathbf{p_i},\mathbf{q_i}) = \sum_{\mathbf{x_f},\mathbf{y_f}}\sum_{\mathbf{x_i},\mathbf{y_y}} e^{i(\mathbf{p_f}\cdot\mathbf{x_f}+\mathbf{q_f}\cdot\mathbf{y_f})} e^{-i(\mathbf{p_i}\cdot\mathbf{x_i}+\mathbf{q_i}\cdot\mathbf{y_i})} \langle 0|NN_i(t,\mathbf{x_f},\mathbf{y_f})NN_j^\dagger(0,\mathbf{x_i},\mathbf{y_i})|0\rangle$$
- The quark-level contraction cost significantly increases (instead of 6-quarks from one source, we have N_{eig} sources for each quark → N_{eig}^4 contractions)
  - But - this also provides a volume averaging at the source (as well as the sink)
  - and also much richer set of correlators/spectrum to analyze

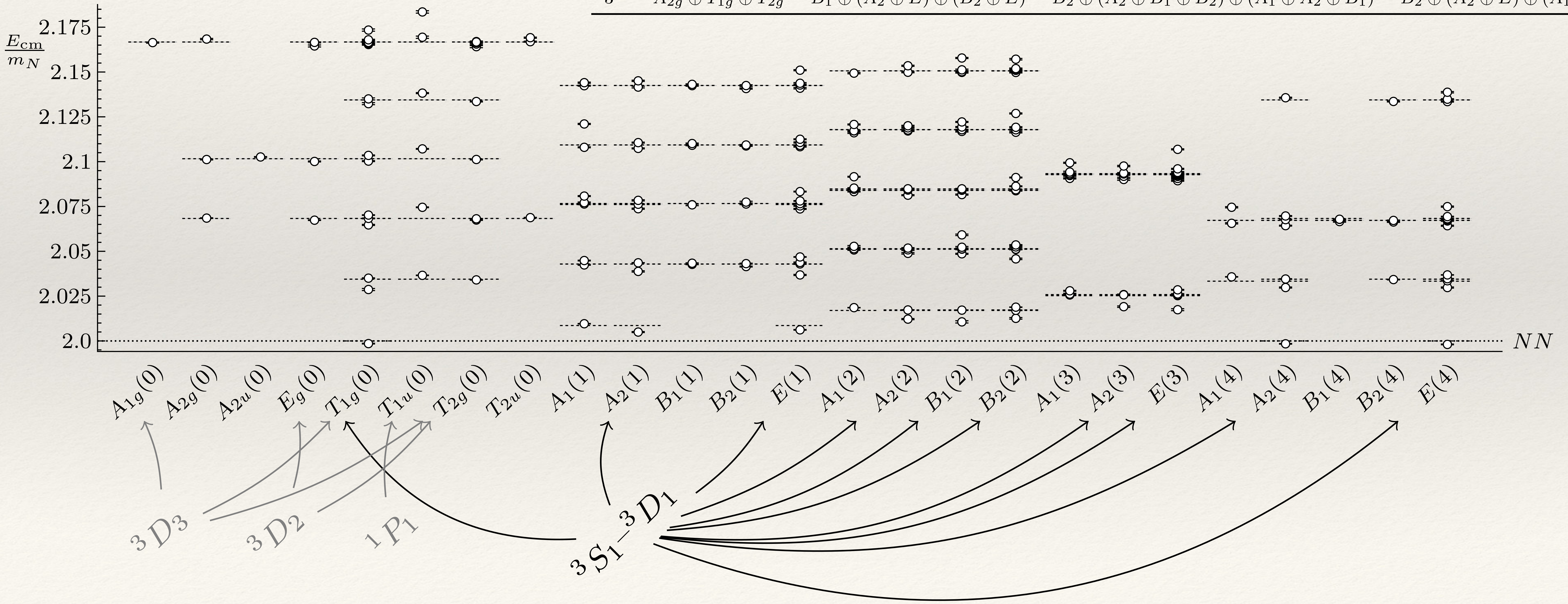
NN with sLapH

arXiv:2009.11825

Mpi~714 MeV

	[000]	[00n]	[0nn]	[nnn]
0^+	A_{1g}	A_1	A_1	A_1
0^-	A_{1u}	A_2	A_2	A_2
1^+	T_{1g}	$(A_2 \oplus E)$	$(A_2 \oplus B_1 \oplus B_2)$	$(A_2 \oplus E)$
1^-	T_{1u}	$(A_1 \oplus E)$	$(A_1 \oplus B_1 \oplus B_2)$	$(A_1 \oplus E)$
2^+	$E_g \oplus T_{2g}$	$(A_1 \oplus B_1) \oplus (B_2 \oplus E)$	$(A_1 \oplus B_2) \oplus (A_1 \oplus A_2 \oplus B_1)$	$E \oplus (A_1 \oplus E)$
2^-	$E_u \oplus T_{2u}$	$(A_2 \oplus B_2) \oplus (B_1 \oplus E)$	$(A_2 \oplus B_1) \oplus (A_1 \oplus A_2 \oplus B_2)$	$E \oplus (A_2 \oplus E)$
3^+	$A_{2g} \oplus T_{1g} \oplus T_{2g}$	$B_1 \oplus (A_2 \oplus E) \oplus (B_2 \oplus E)$	$B_2 \oplus (A_2 \oplus B_1 \oplus B_2) \oplus (A_1 \oplus A_2 \oplus B_1)$	$B_2 \oplus (A_2 \oplus E) \oplus (A_1 \oplus E)$

only P_{tot}=0 energy levels shown



NN with sLapH

arXiv:2009.11825

Mpi~714 MeV

- In this first work - we focus on states below the t-channel cut which also have only predominant S-wave interactions
- Given the spectrum and resulting phase-shift values, we perform an effective range expansion analysis

$$q\cot\delta(q) = -\frac{1}{a} + \frac{1}{2}r_0 q^2 + \frac{1}{6}r_1 q^4 + \cdots$$

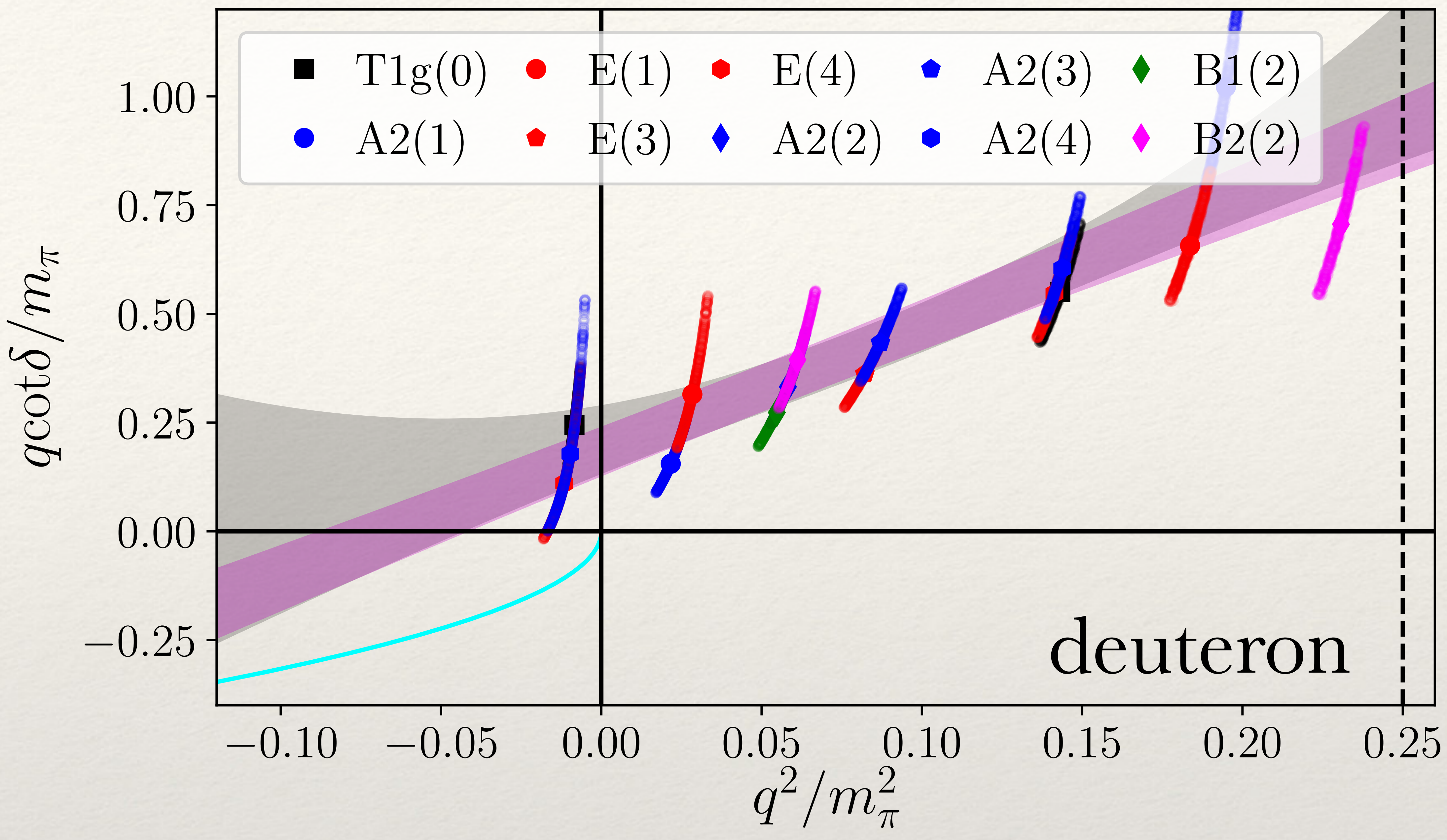
$$m_\pi a = -5.5(1.6), \quad m_\pi r_0 = 5.82(.71)$$

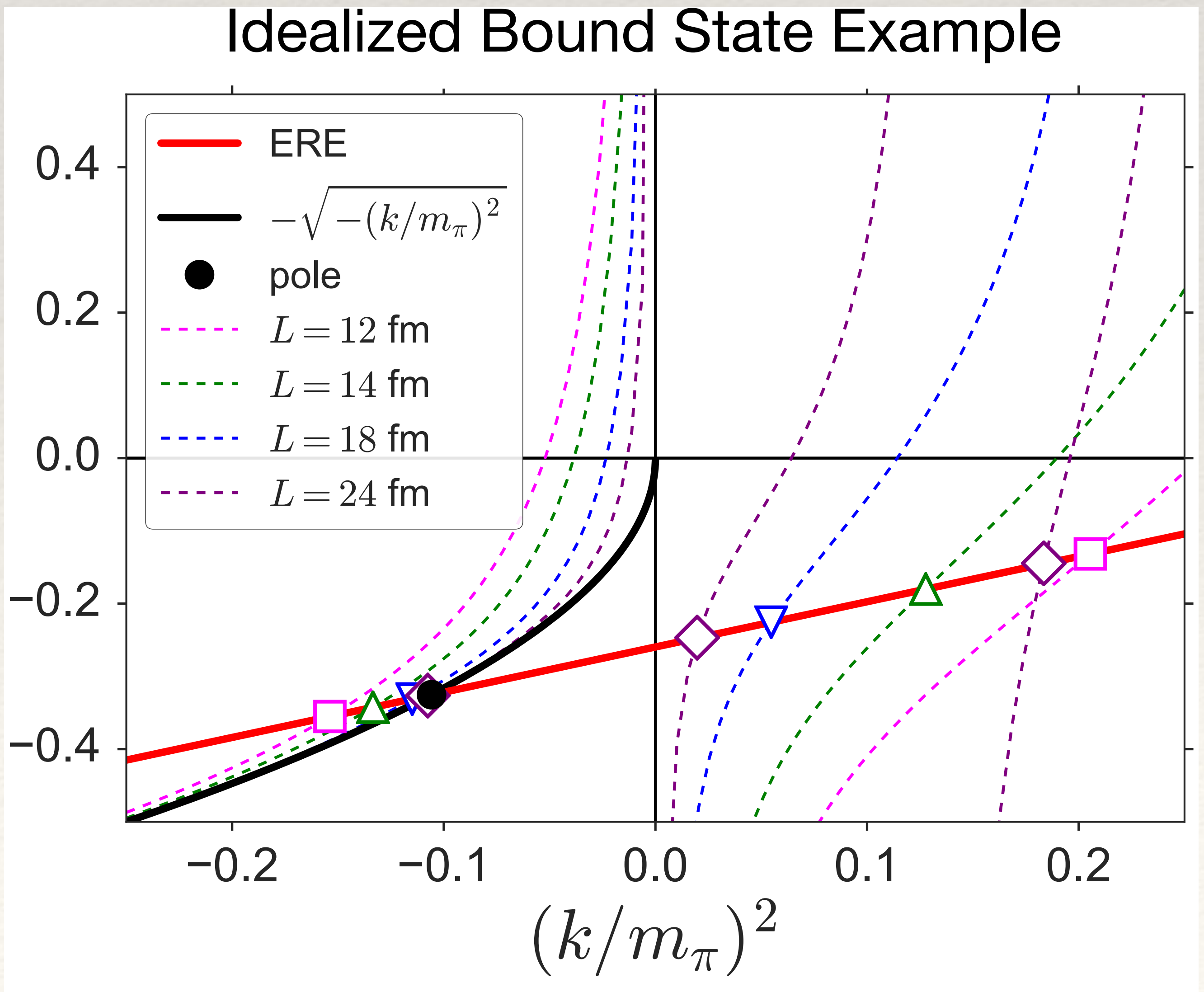
- A bound state solution requires $q\cot\delta(q)\Big|_{q=0} < 0$ and a slope < tangent to $-\sqrt{-q^2}$
- We find a virtual bound state (like dineutron) - a purely imaginary solution with negative sign

$$\frac{q_-^{\text{deuteron}}}{m_\pi} = -i\,0.132(32)$$

- We can infer the size of the potential from causality and unitarity: Wigner PRD 98 (1955), Phillips and Cohen PLB 390 (1997)

$$r_0 \leq 2\left[R - \frac{R^2}{a} + \frac{R^3}{3a^2}\right] \qquad m_\pi R \gtrsim 2.0, \quad R \gtrsim 0.55\text{ fm}$$





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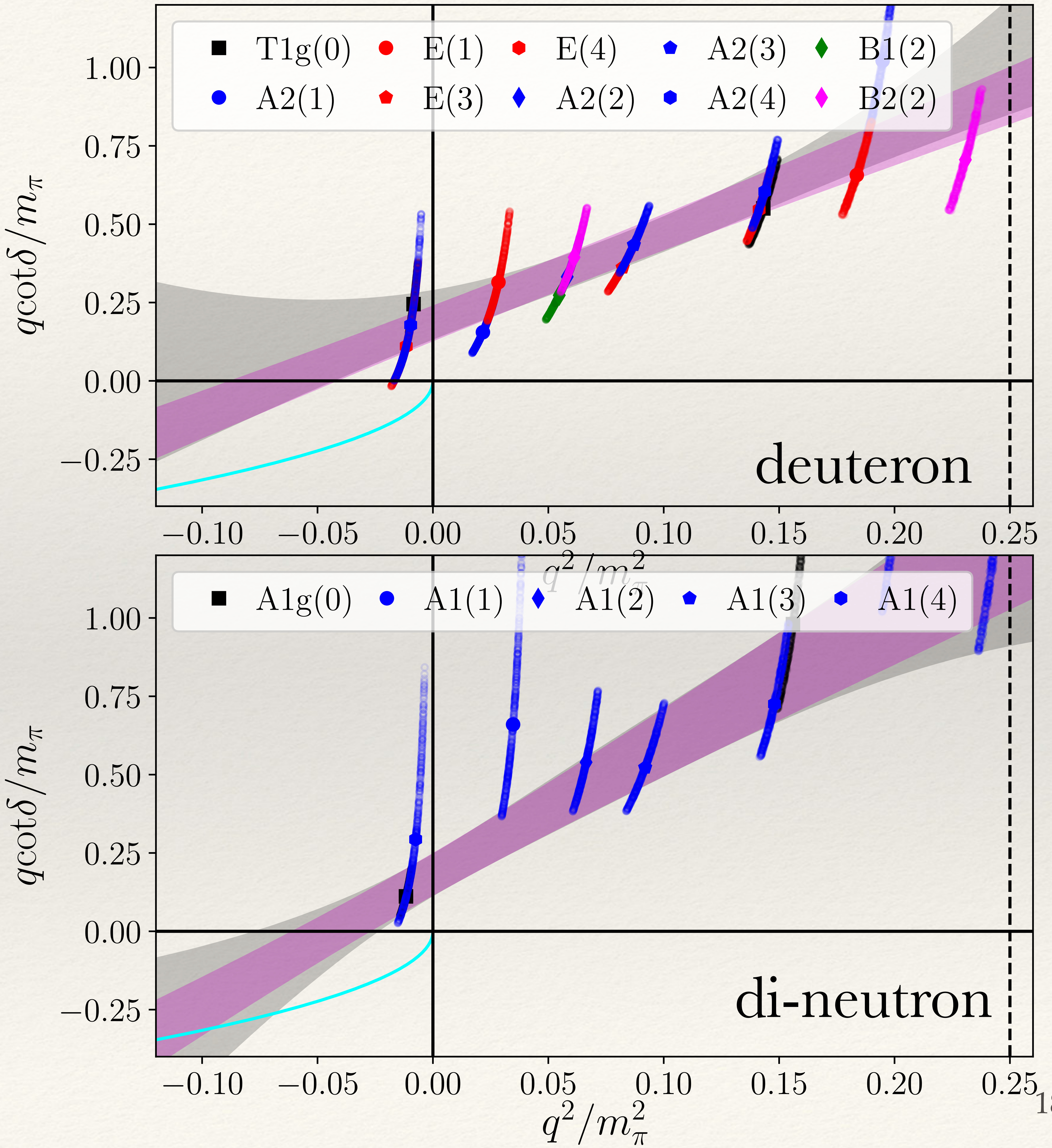

Comparing with NPLQCD

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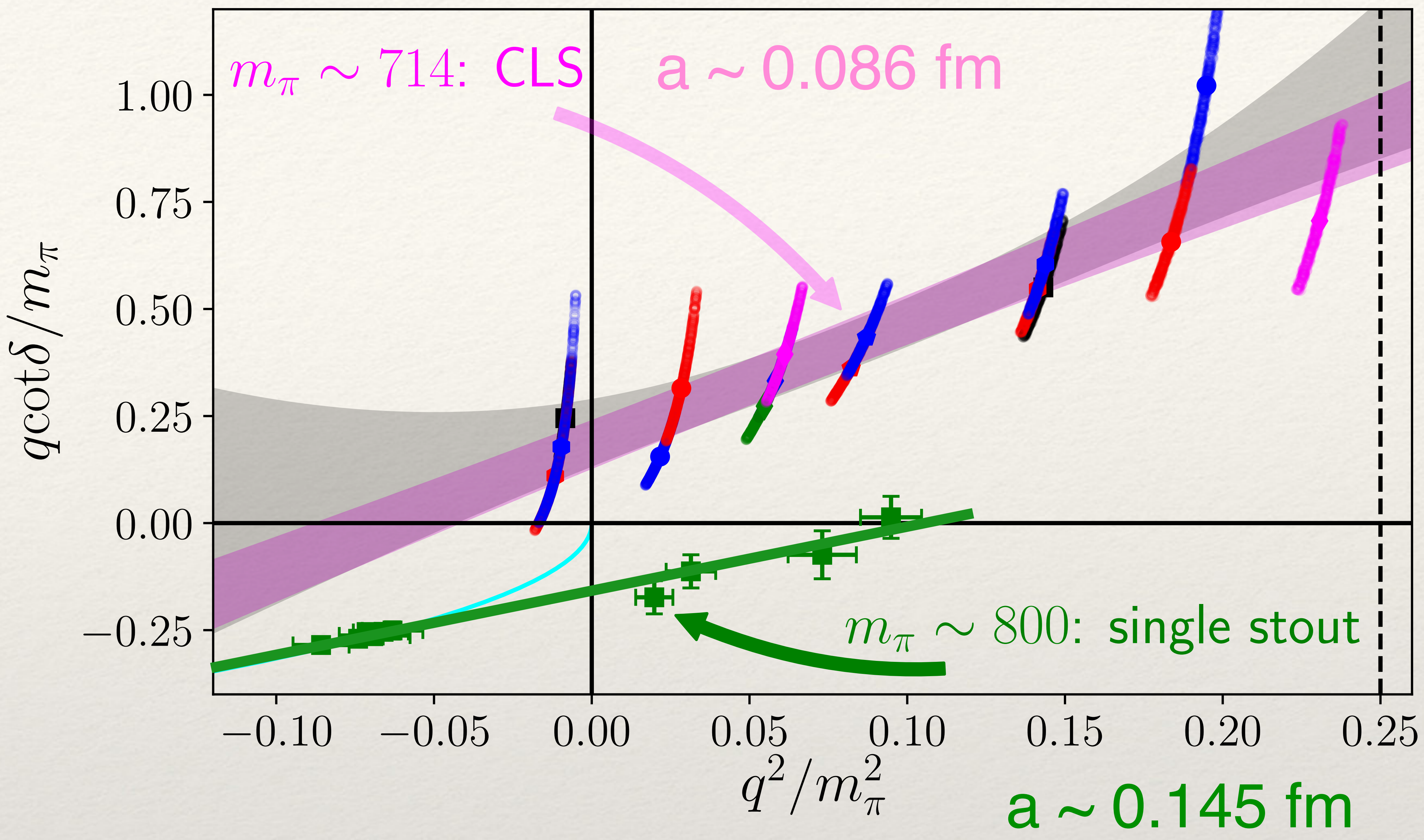
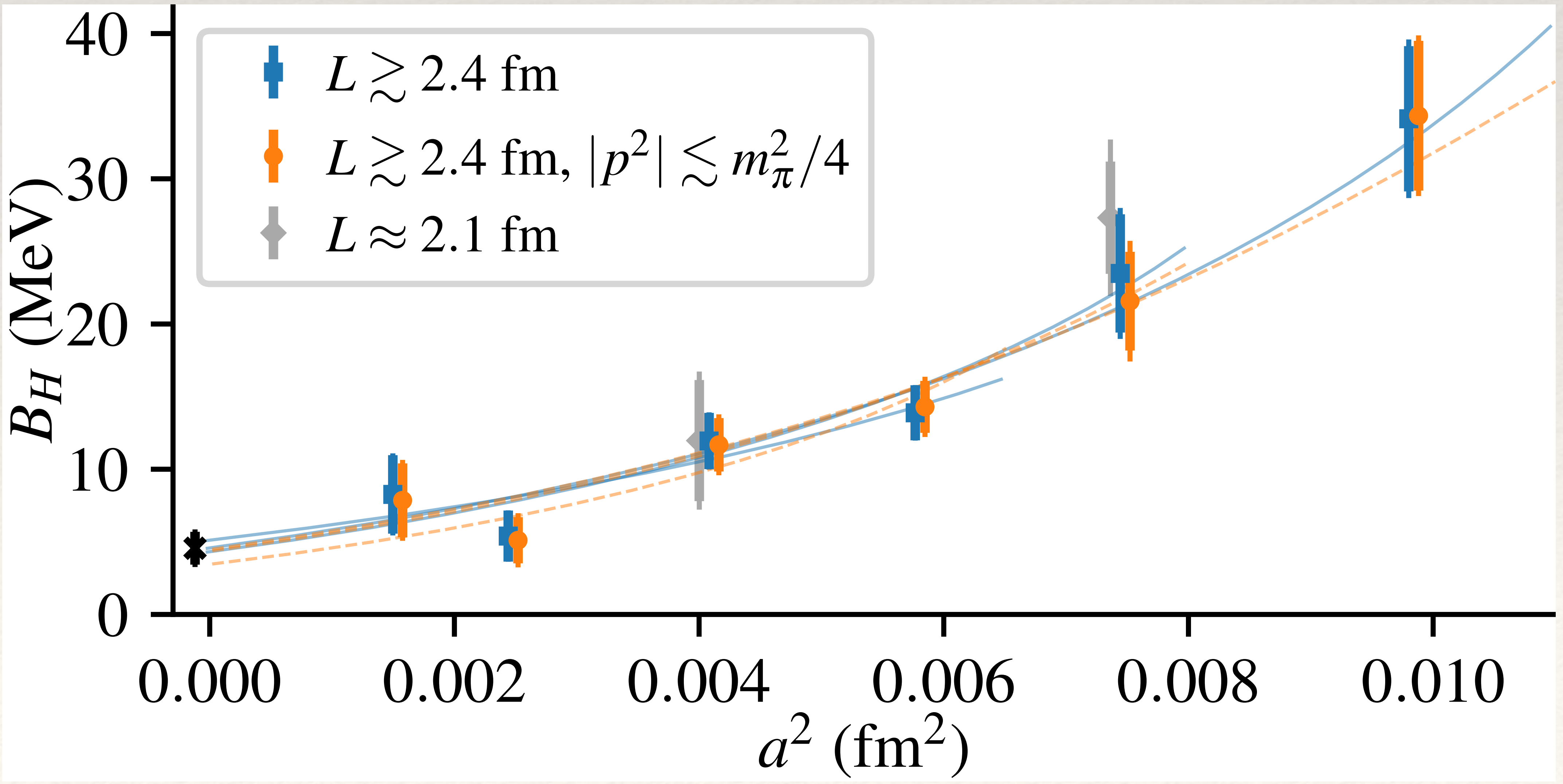
      But see Green et al [Mainz] PRL 127 (2021) [arXiv:2103.01054]
      800% correction to the binding energy observed for H-dibaryon at SU(3) flavor symmetric point





In the works

- At Mpi ~ 714 MeV, a ~ 0.086 fm @ SU(3) flavor symmetric point
  - We increased our statistics by a factor of ~8
    Analyzing higher partial waves and S-D mixing (developing the technology pipeline)
    Fitting spectrum results with $HOBET_{FV}$ (K. McElvain and W. Haxton)
  - We are adding a hexaquark operator to our basis to see if it modifies the spectrum
  - Performing the NPLQCD, CalLat and HAL QCD calculations on the same gauge configurations
    - isolate the method as the systematic uncertainty which can cause results to vary (postpone worrying about continuum extrapolation till later)
- We are running the same calculation on an ensemble with Mpi ~ 200 MeV and a ~ 0.064 fm
  - pi-N scattering and Delta resonance is being prepared for publication
  - The Y-N results look promising
  - The N-N results need more statistics

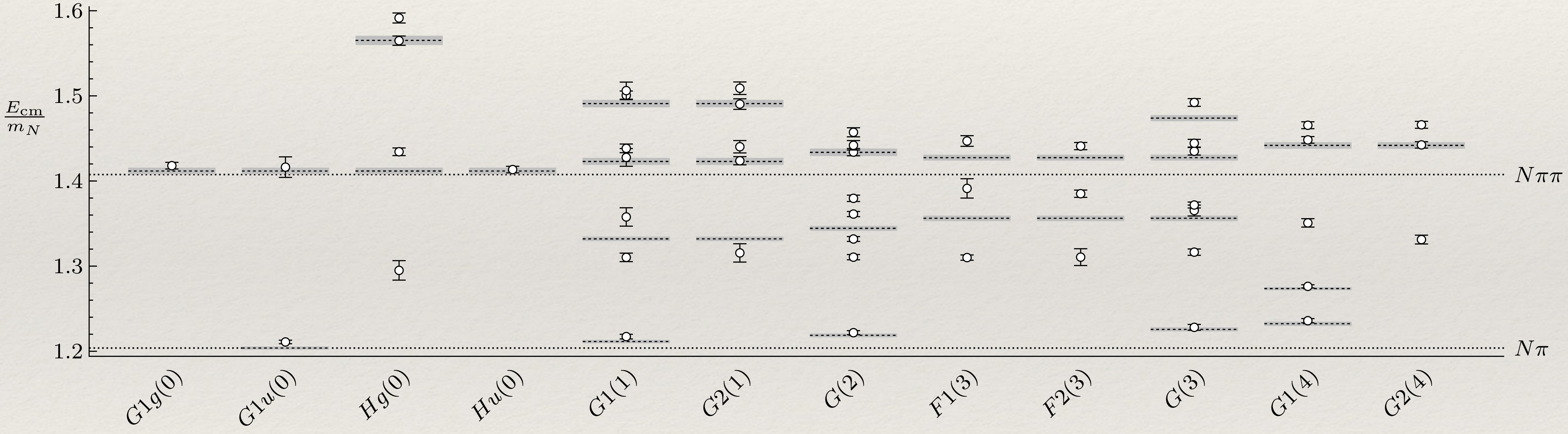
Why am I optimistic of parity violating calculations soon?

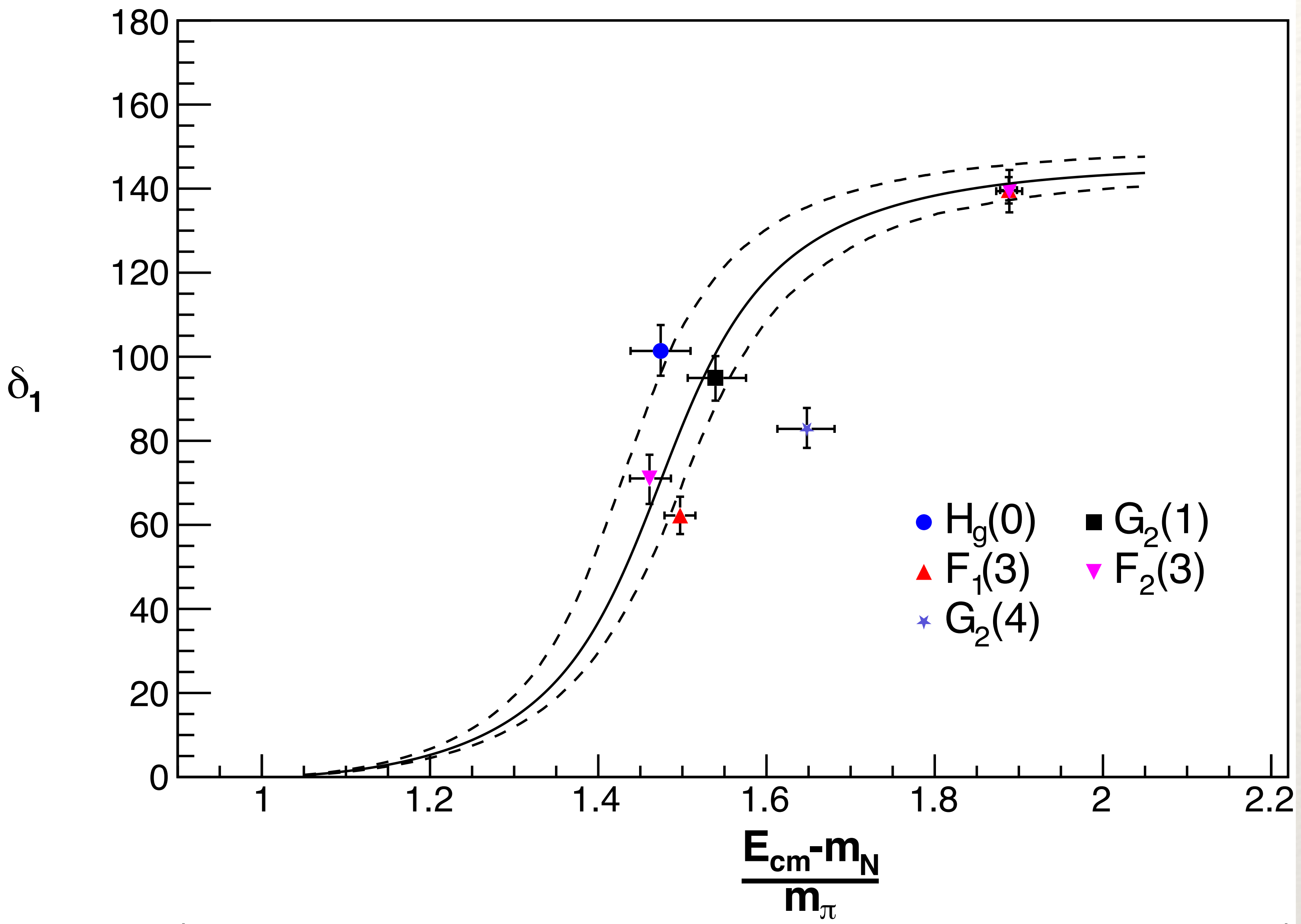
- See the next 2 talks!
  - Chien Yeah Seng - formal developments
  - Marcus Petschlies - numerical calculation for $\Delta I = 1$

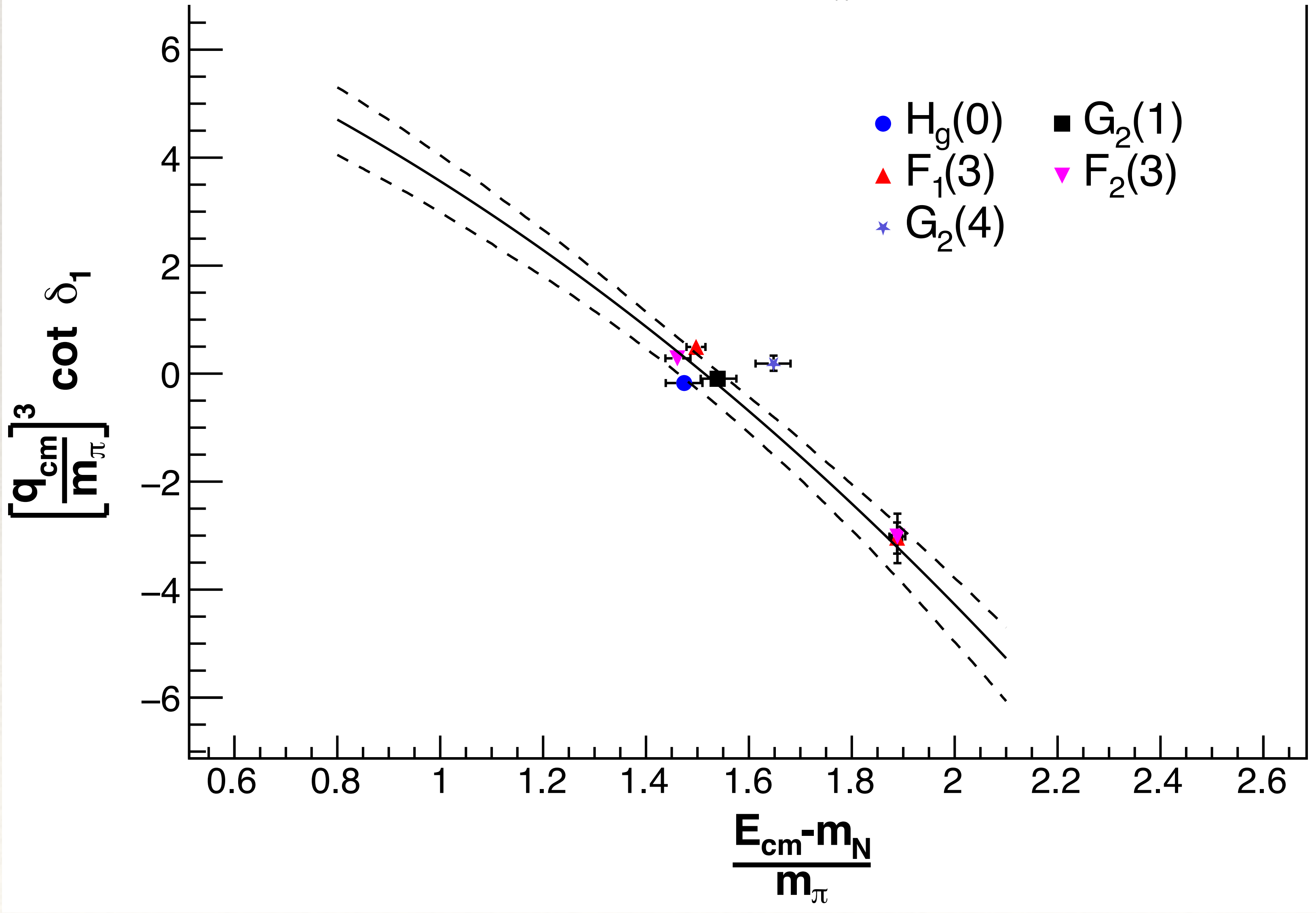
Why am I optimistic of parity violating calculations soon?

- The use of variational methods for NN and pi-N is now a reality with Mpi ≳ 200 MeV

Preliminary I=3/2 pi-N scattering @ Mpi ~ 200 MeV (Bulava et al)

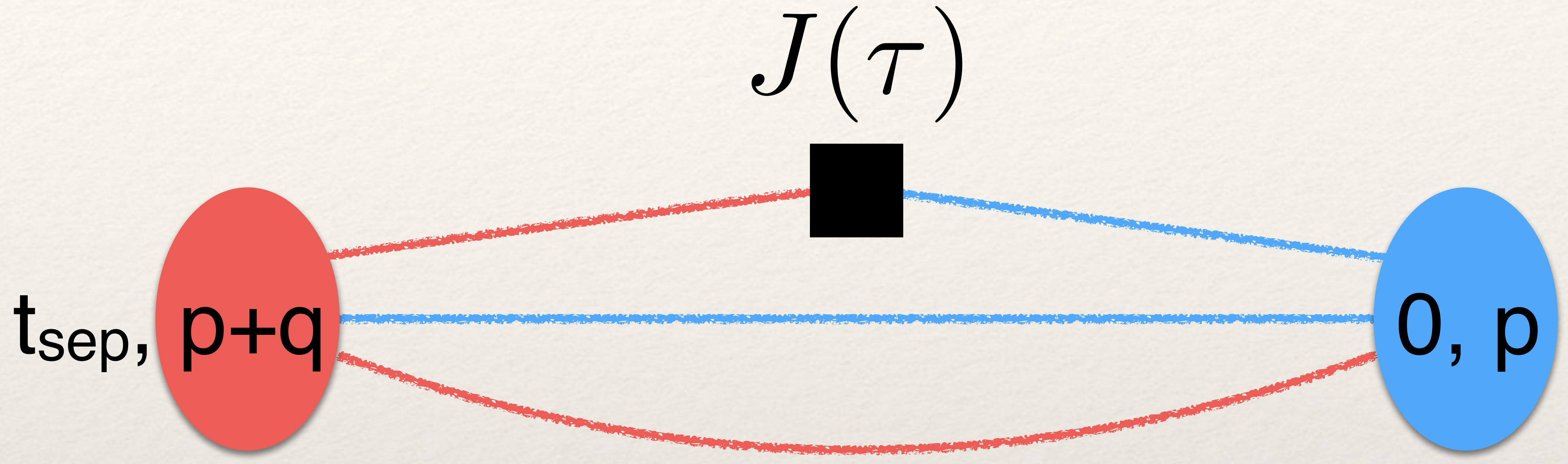






Why am I optimistic of parity violating calculations soon?

- The use of variational methods allows for new methods to compute matrix elements and form factors
  - For each $0 < \tau <$ t_{sep}:
    - point source at current
    - solve propagator
    - tie this prop to source and sink in momentum space



- If this method proves fruitful, the technology is easily adaptable to performing 2-nucleon matrix elements of quark bi-linear and 4-quark operators
  - We expect to know this year how well the method works

Conclusions

- We have had a “breakthrough” in LQCD calculations of NN interactions - utilizing variational methods that enable momentum space creation and annihilation operators
- I believe this means we will see earnest calculations of hadronic parity violation in the next few years
  - N→N-pi (Sen, Petschlies, Schlage, Urbach)
  - NN→NN
- These LQCD calculations in A ≤ 3 systems can be analyzed in concert with experimental results
  - LQCD can provide a few orthogonal inputs to understanding the low-energy processes and EFT
  - Determine LECs from LQCD - then predict more complicated observables
    - $\Delta I=2$ - probably easiest - need NN scattering and matrix elements
    - $\Delta I=1$ - next easiest - need pi-N scattering and matrix elements
    - $\Delta I=0$ - very challenging…

Conclusions

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- I believe this means we will see earnest calculations of hadronic parity violation in the next

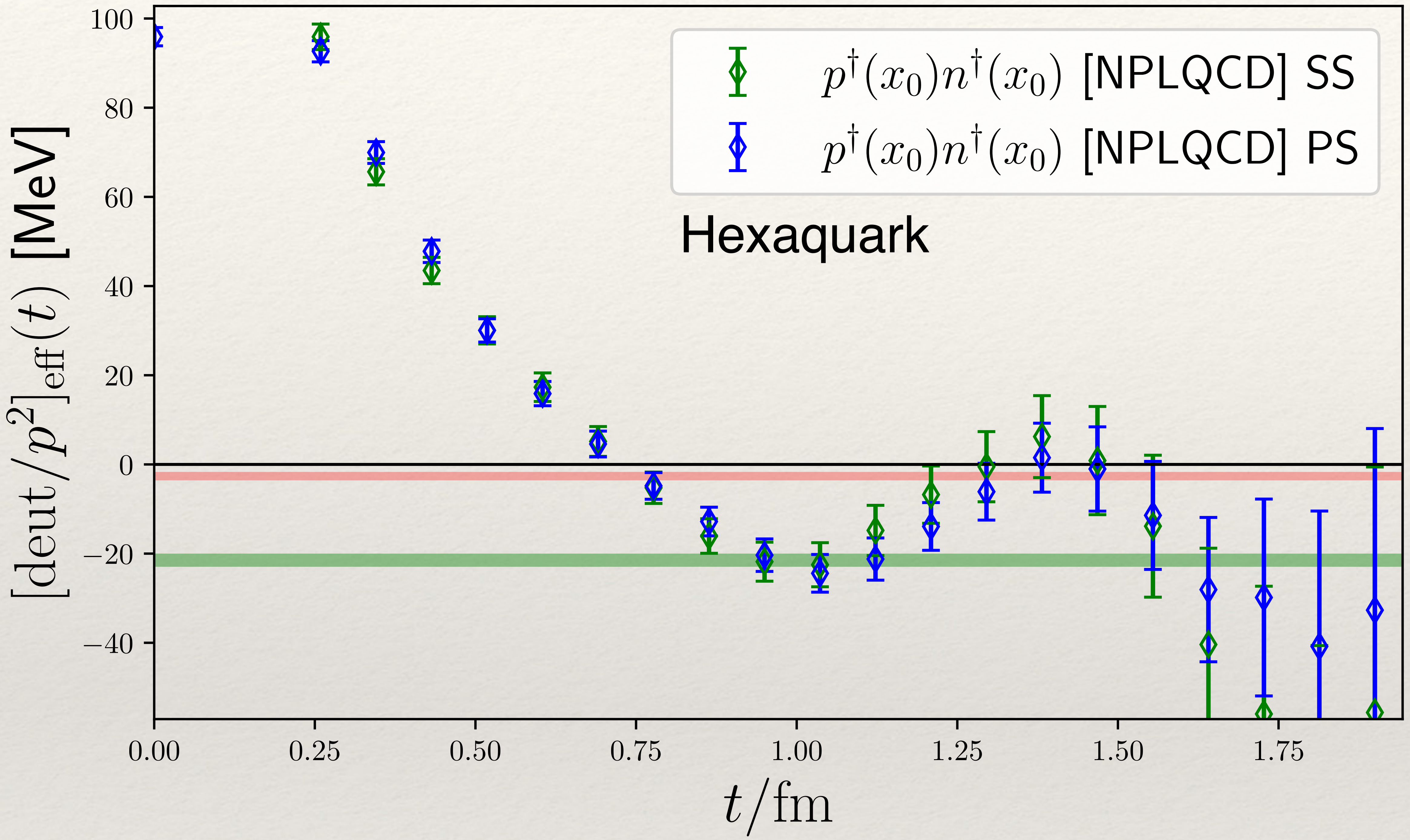
What set of N and NN observables are most useful to determine for constraining the PV LECs?

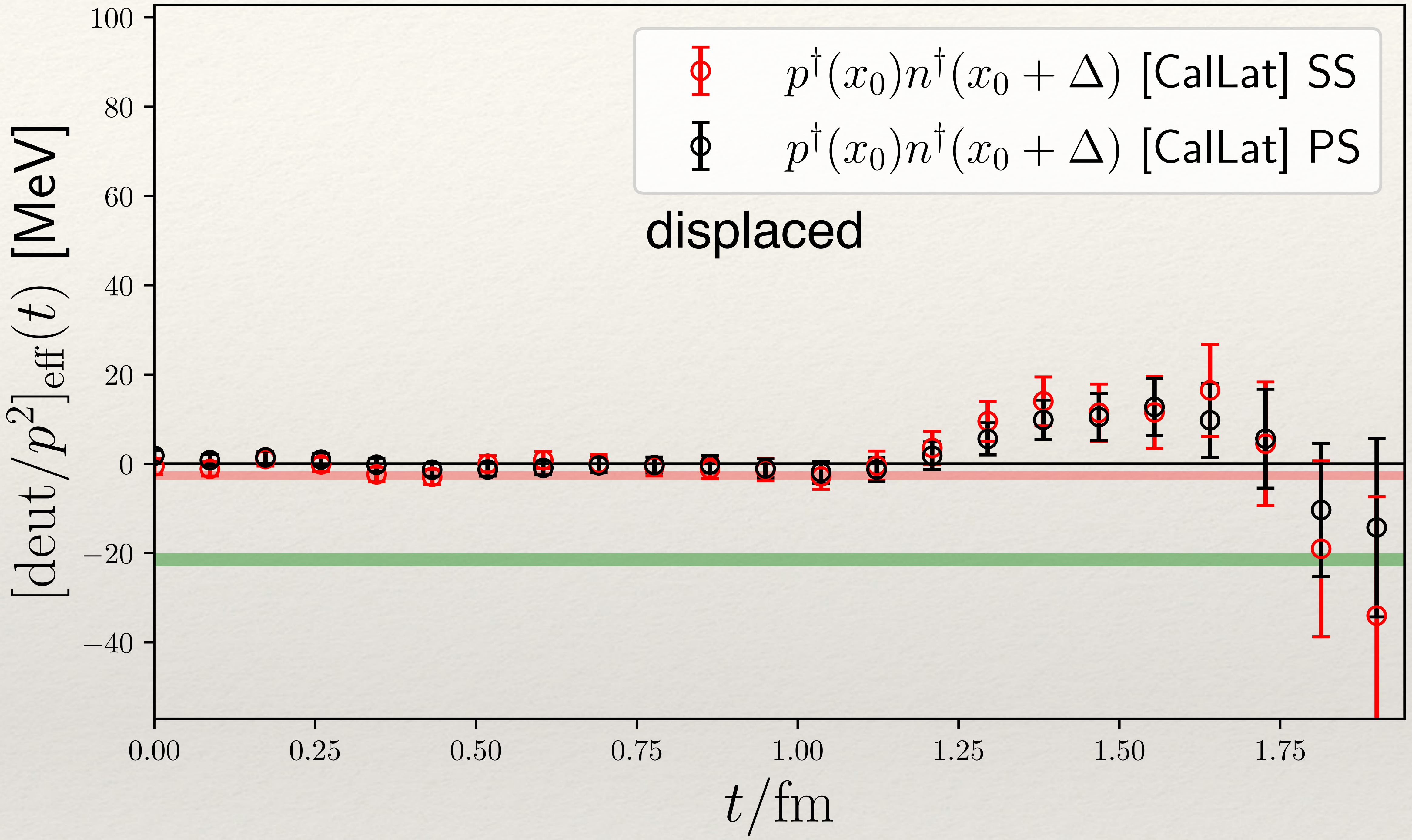
- These LQCD calculations in $A \leq 3$ systems can be analyzed in concert with experimental results
  - LQCD can provide a few orthogonal inputs to understanding the low-energy processes and EFT
  - Determine LECs from LQCD - then predict more complicated observables
    - $\Delta I=2$ - probably easiest - need NN scattering and matrix elements
    - $\Delta I=1$ - next easiest - need pi-N scattering and matrix elements
    - $\Delta I=0$ - very challenging…

Thank You

Preponderance of evidence: NPLQCD like and CalLat like

- Preliminary results on same Mpi~714 MeV, a~0.086fm ensembles





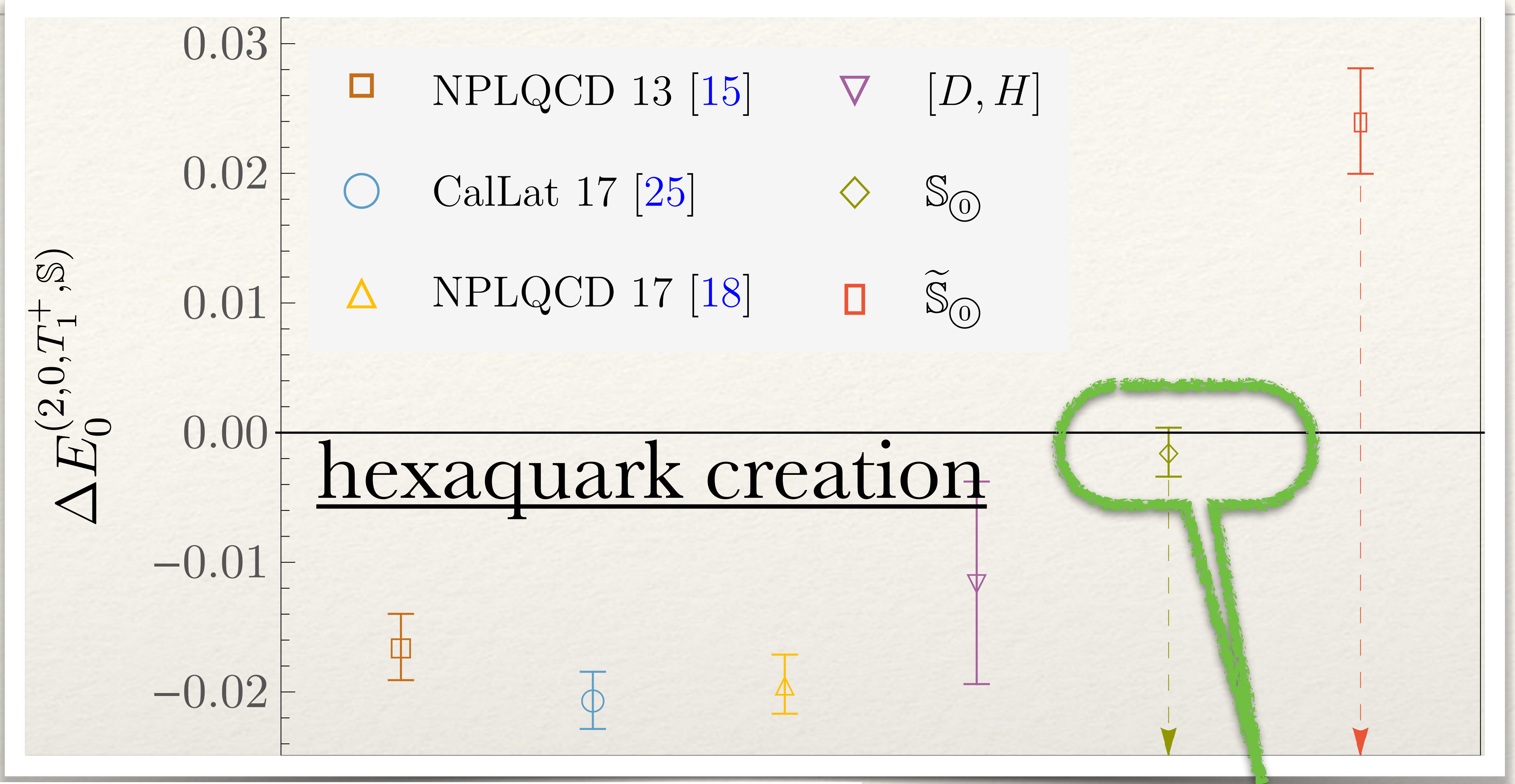
- green band: NPLQCD deep binding at Mpi~800
  red band: sLapHnn energy shift with momentum space creation and annihilation, then GEVP (variational)

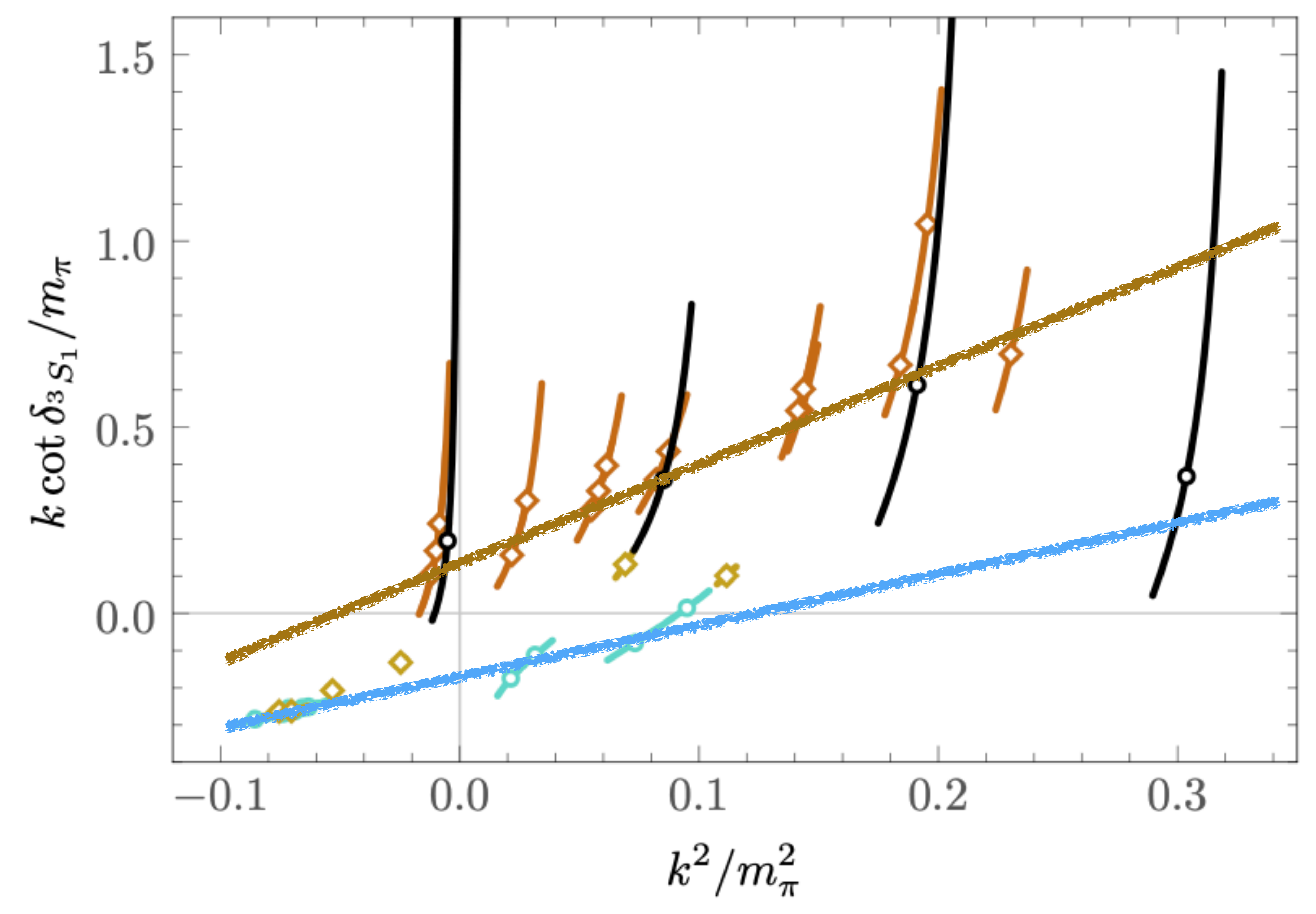
- $N^\dagger(t_0, x_0)N^\dagger(t_0, x_0)$ seems favor deep bound state (for point-nucleons, uniform coupling to all NN momentum modes)

- $N^\dagger(t_0, x_0)N^\dagger(t_0, x_0 + \Delta)$, excited states in NN and N seem to (nearly) perfectly exactly cancel

New NPLQCD work - arXiv:2108.10835

- Recent NPLQCD work - Mpi~800 MeV “momentum sparsening” [1908.07050] to do momentum-space creation operators
- They conclude that existence of deep bound state or not is inconclusive
- Phase-shift analysis inconsistent between old (blue) and new (black)
- If a state couples to one (or more) operators, adding more operators should not drag the state around
- shifting spectrum indicative of previously deficient basis





- hexaquark and momentum space creation
- this level does not change when hexaquark is removed, or more/less momentum states used

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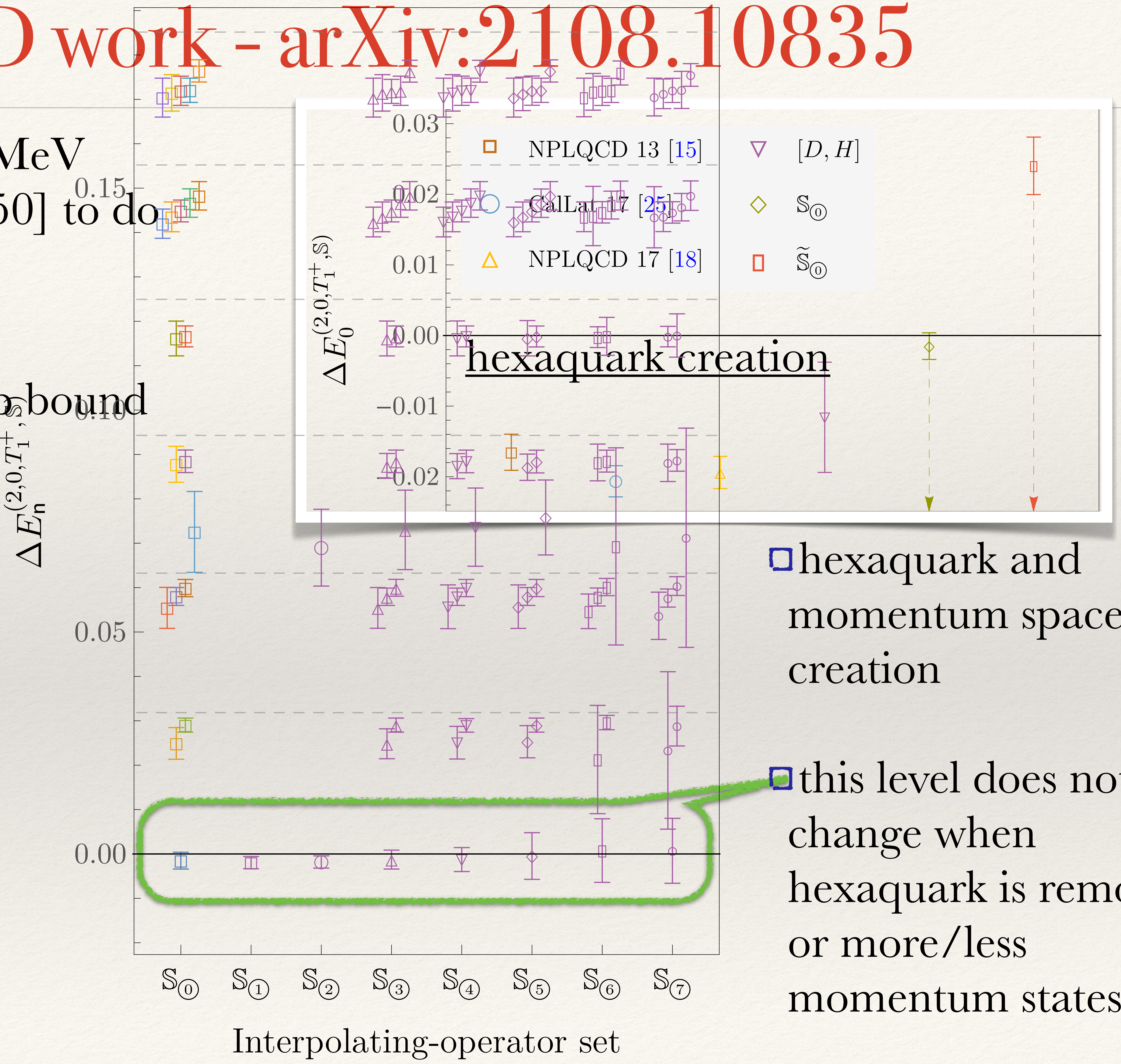
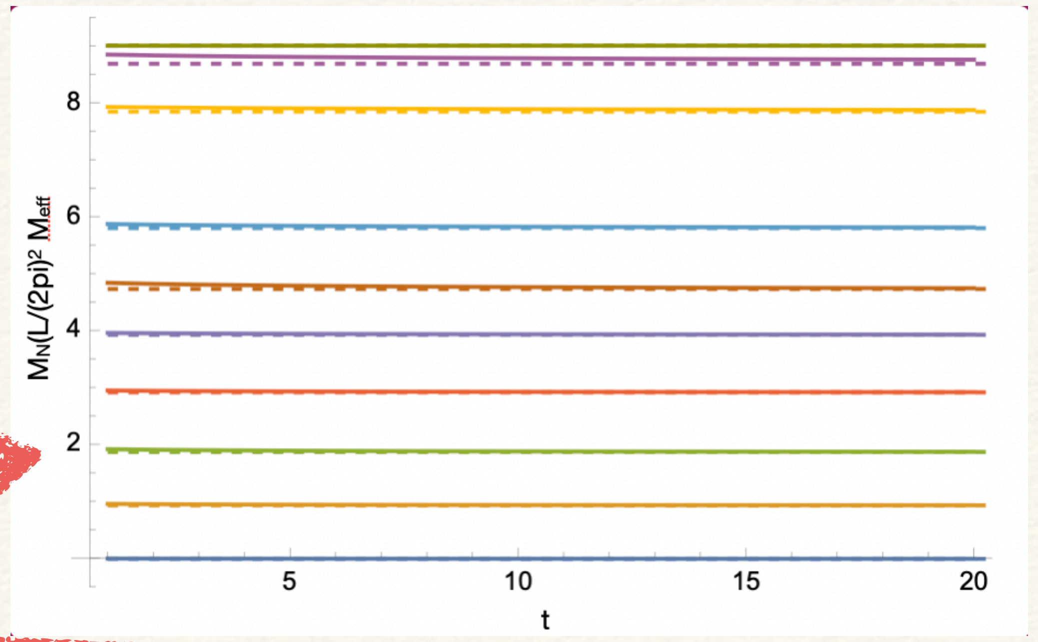
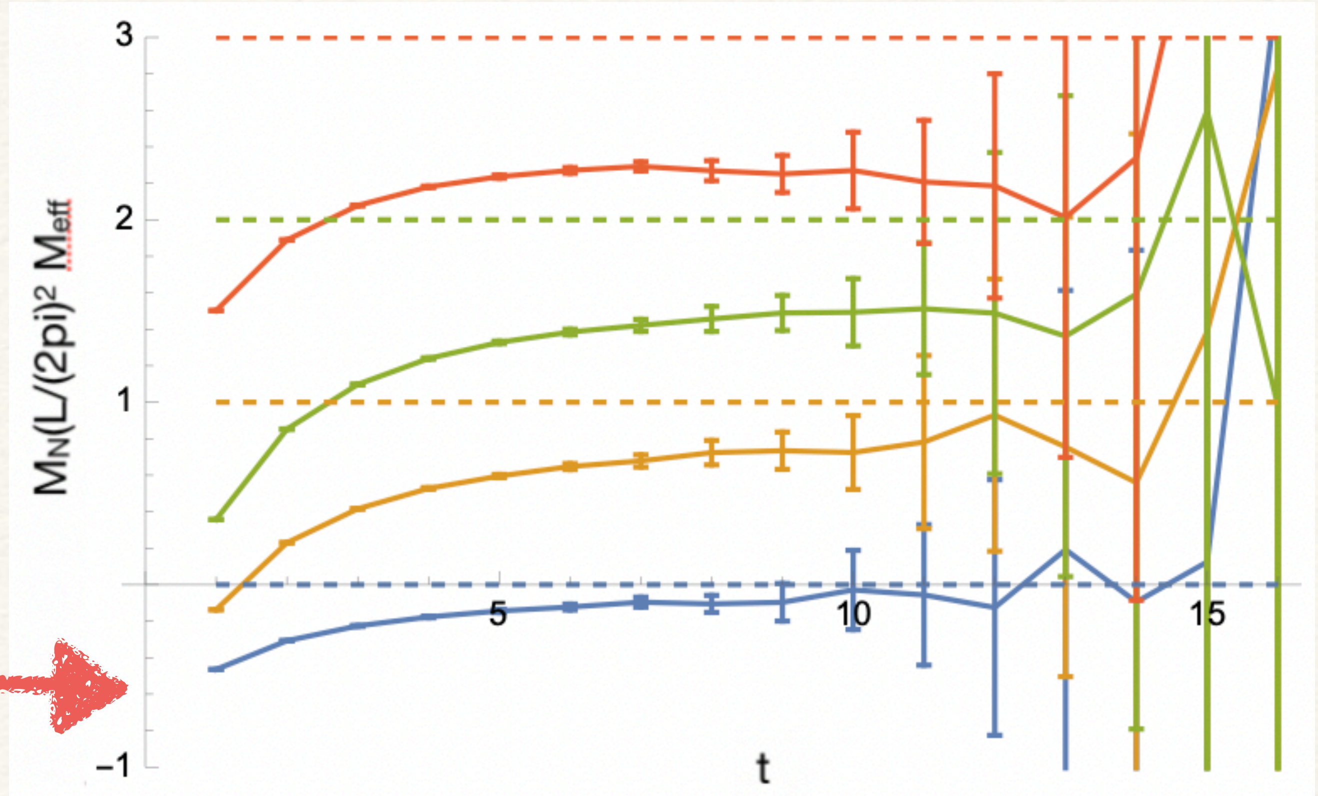


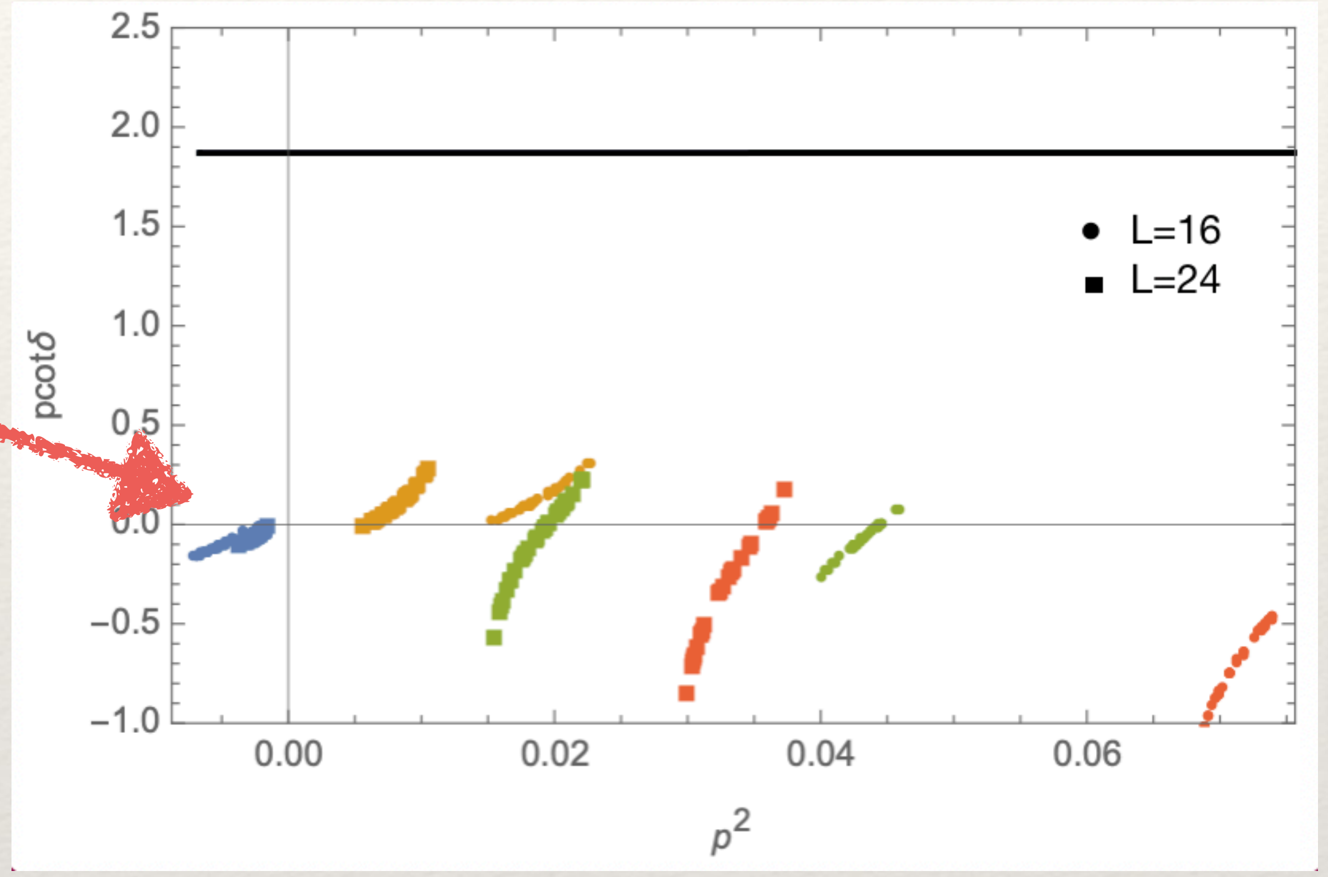
- hexaquark and momentum space creation
- this level does not change when hexaquark is removed, or more/less momentum states used

❑ pion-less EFT (no inelastic excited states)

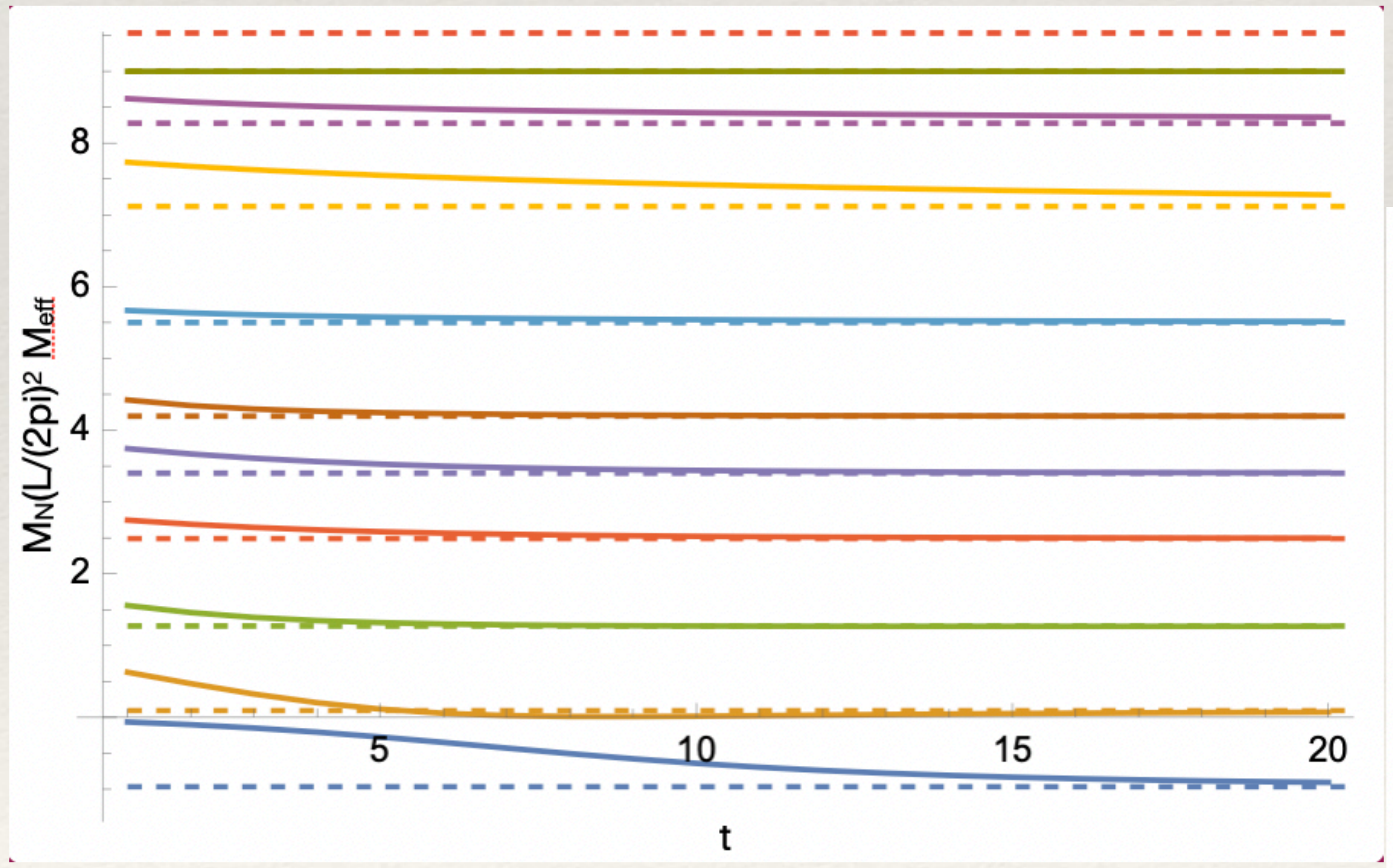
- ❑ system without a bound state:
  - ❑ momentum space operators: reproduces spectrum
  - ❑ hexaquark operator: effective masses all “pulled down”
  - ❑ observed volume-independence of ground state

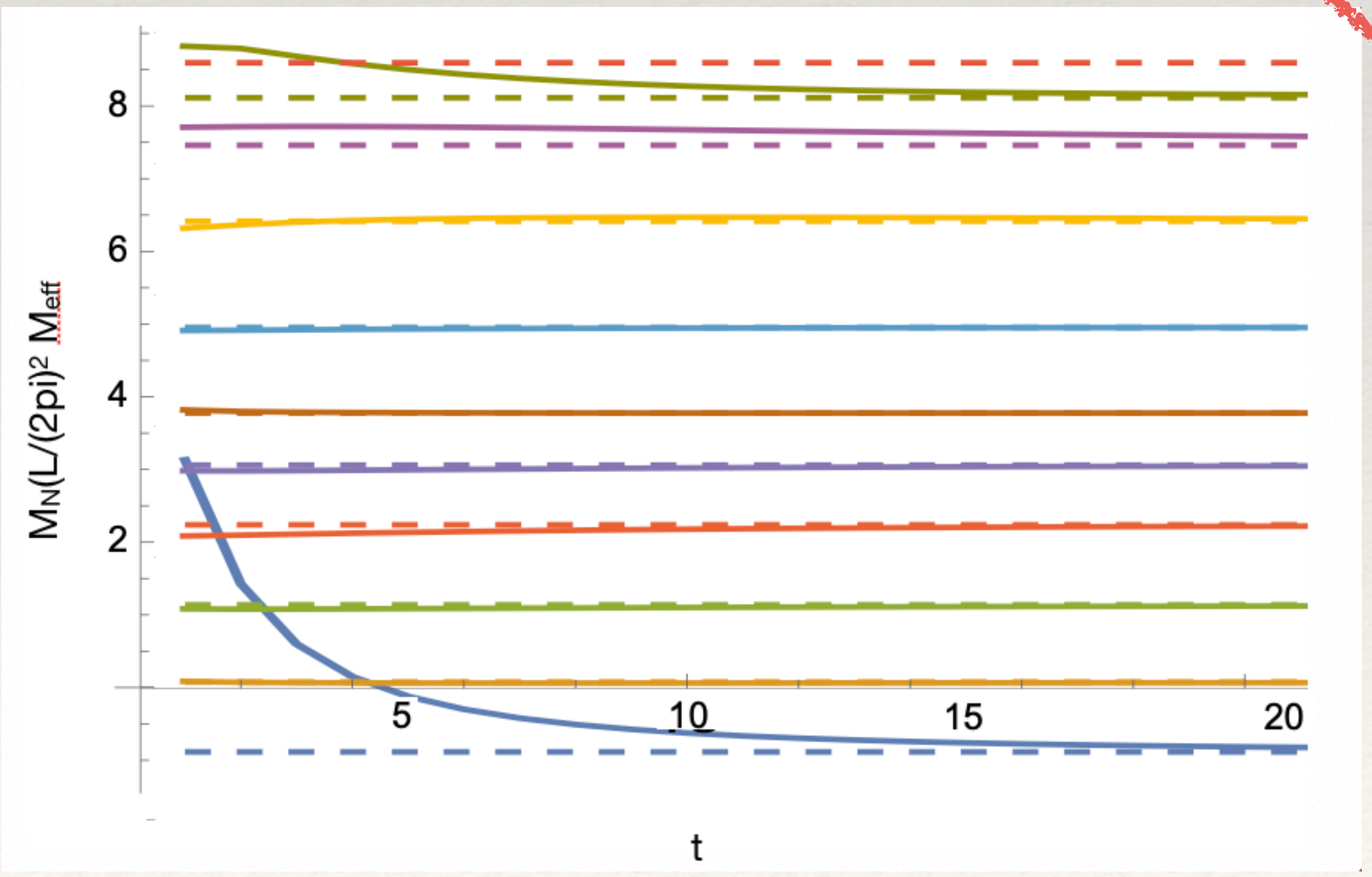


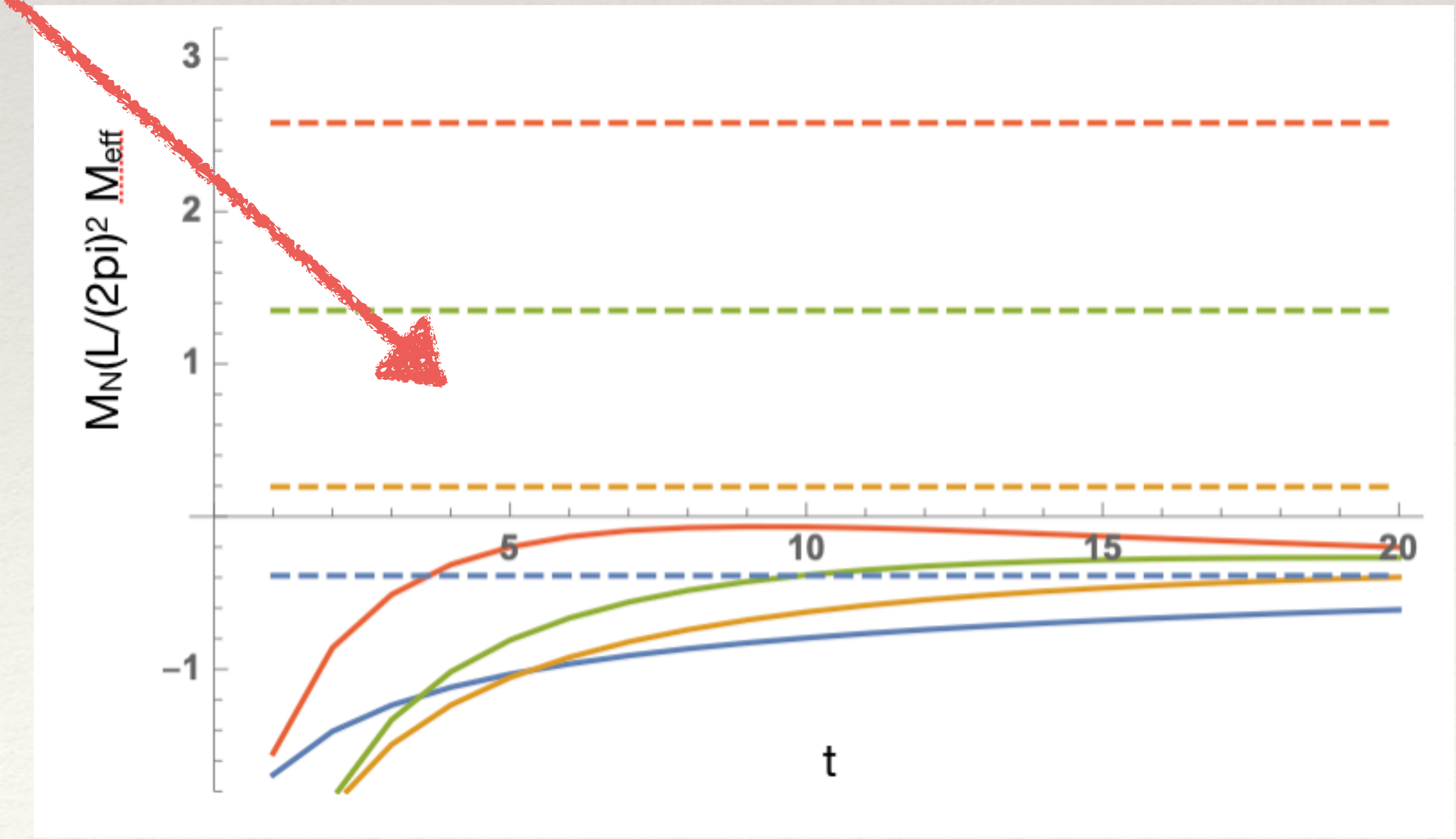




- ❑ system with bound state:
  - ❑ momentum space operators: reproduces spectrum
  - ❑ addition of hexaquark: does not improve spectrum
  - ❑ hexaquark operator: identifies bound state - all other states also collapse to ground state







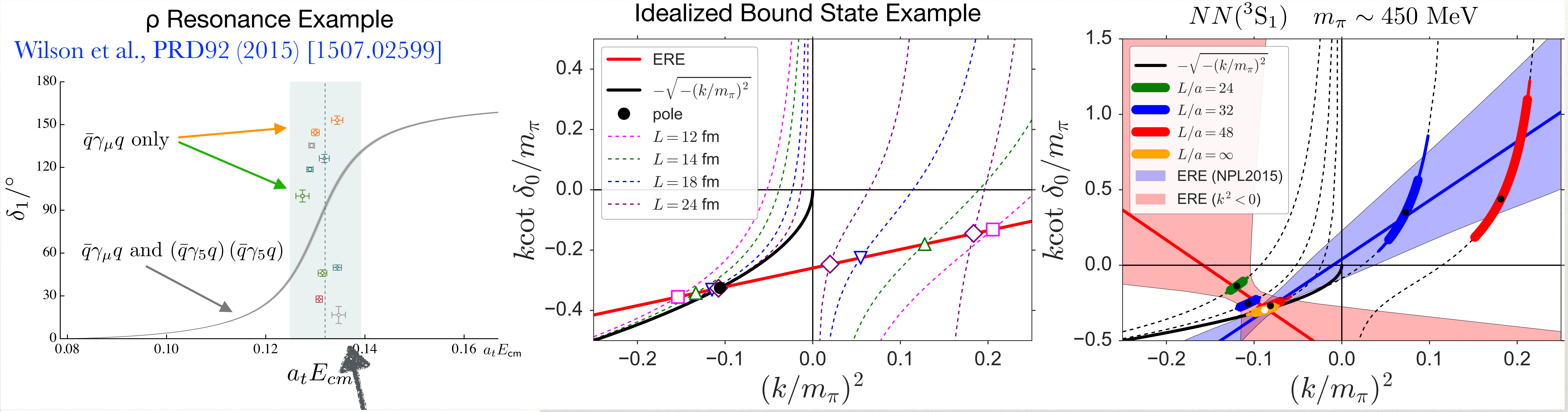
Nicholson et al, Latt2021
[2112.04569]

Two-nucleon controversy/discrepancy

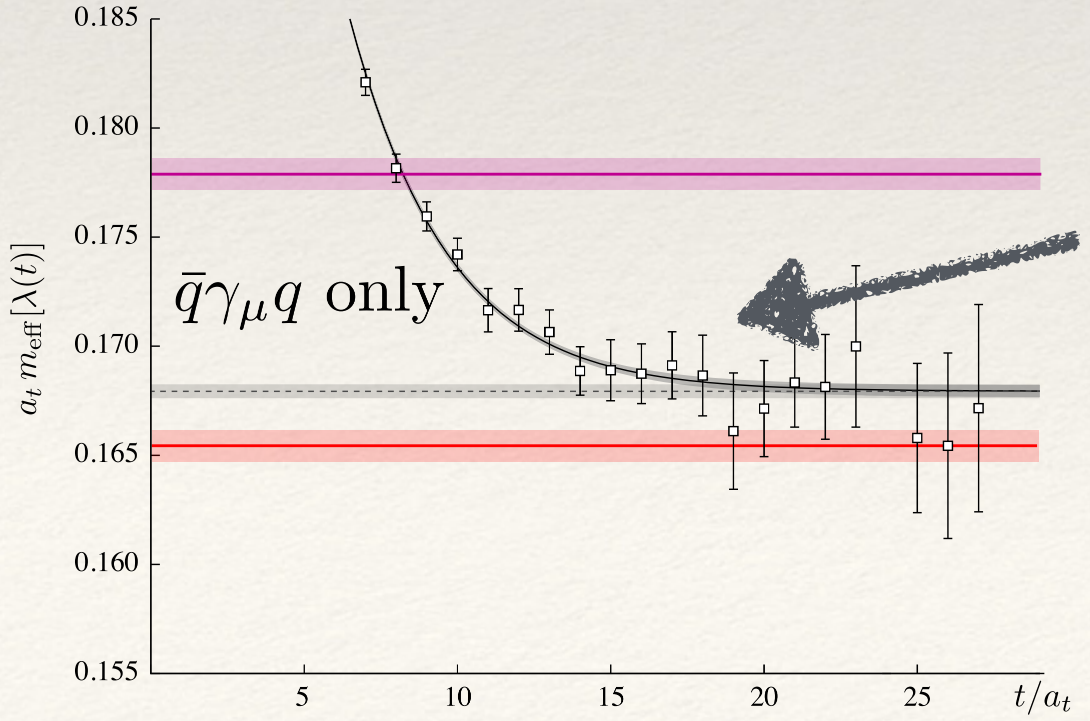
Towards grounding nuclear physics in QCD
C. Drischler, W. Haxton, K. McElvain,
E. Mereghetti, A. Nicholson, P. Vranas, AWL
PPNP 121 (2021) [arXiv:1912.03580]

- HAL QCD Consistency Checks [1703.07210]

NPLQCD PRD 92 (2015) [1508.07583]



False energy levels can be detected from not obeying expectations from Lüscher



seemingly healthy effective mass (gray) but does not follow Breit-Wigner

True energy levels must

- Follow the "Lüscher lines" (dashed curves)
- Have correct sign for pole of residue slope of ERE less than slope of bound-state curve, $-\sqrt{-(k/m_\pi)^2}$

- InConsistency of the below and above threshold ERE
- Above-threshold ERE crosses bound-state curve with too large of a slope
- These results have a clear systematic uncertainty issue
- See updated result: 2009.12357

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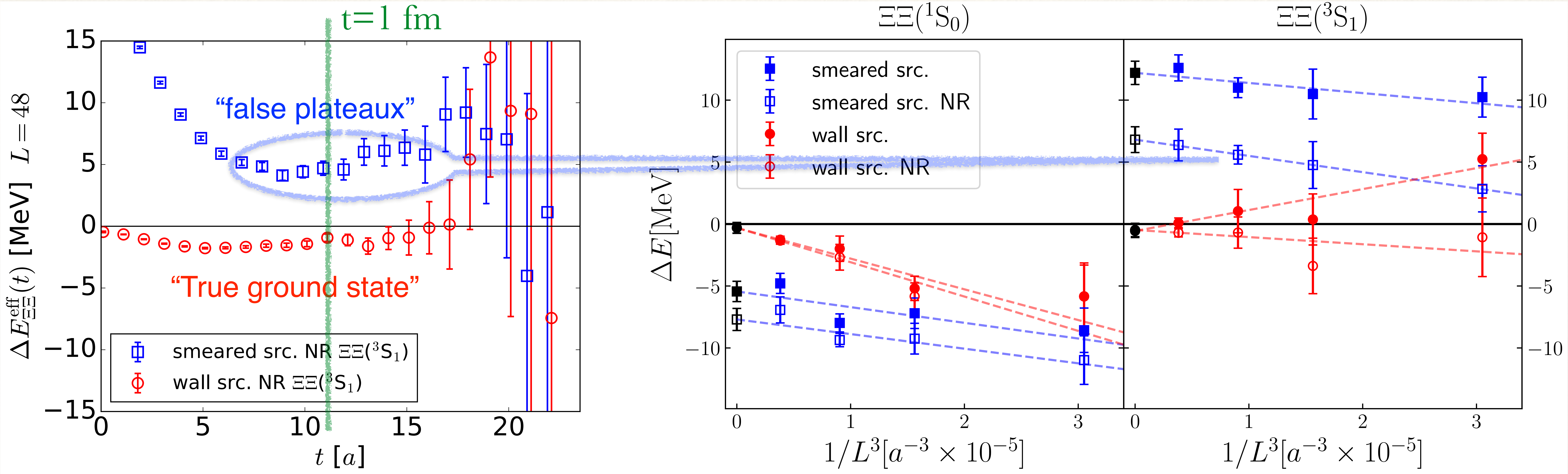
- HAL QCD [1607.06371] - issue with local, gaussian smeared quark source creation operators
  They show that the extracted spectrum depends upon the creation operator



Whether bound or scattering, attractive interactions → ΔE < 0

Bound states have non-vanishing energy as L → ∞

Scattering states have energies that must vanish as L → ∞

$$\Delta E = E - 2M \approx -\frac{4\pi a}{ML^3}\left[1 + \mathcal{O}\left(\frac{a}{L}\right)\right]$$

Two-nucleon controversy/discrepancy

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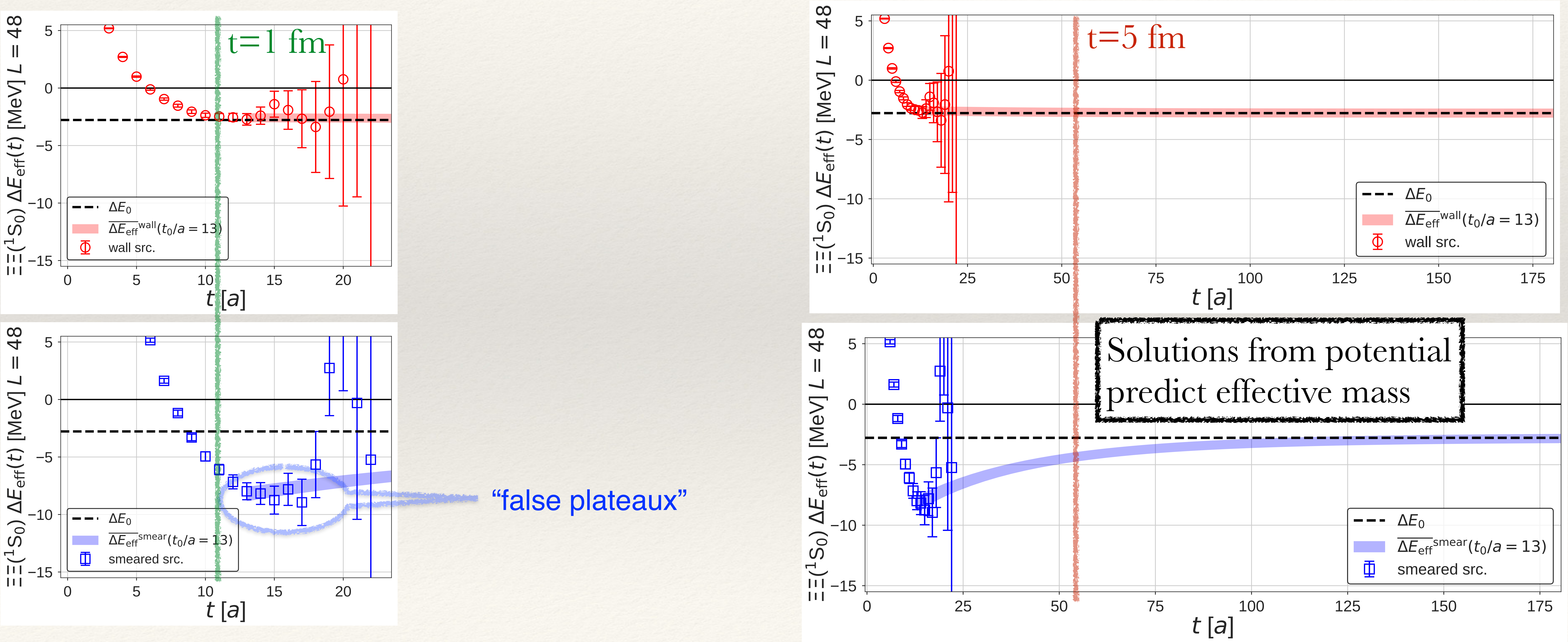
- HAL QCD Potential/Lüscher Consistency [1812.08539]

  These issues led HAL QCD to speculate that we (hexa-quark creation ops) are seeing a false-plateaux generated by linear combinations of *elastic scattering states*



NN with sLapH

arXiv:2009.11825

Mpi~714 MeV

- "Traditional" method: $C_{NN}(t,\mathbf{p}+\mathbf{q}) = \sum_{\mathbf{x}}\sum_{\mathbf{y}} e^{i\mathbf{p}\cdot\mathbf{x}} e^{i\mathbf{q}\cdot\mathbf{y}} \langle 0|N(t,\mathbf{x})N(t,\mathbf{y})N^\dagger(0,\mathbf{0})N^\dagger(0,\mathbf{0})|0\rangle$
- Alternatively - one can solve quark propagators from the eigenvectors of the 3D smearing kernel that is typically used (instead of one propagator per source for many sources) [arXiv:0905.2160]
  - This allows one to construct momentum-based creation operators
  - The quark-level contraction cost significantly increases (instead of 6-quarks from one source, we have N_{eig} sources for each quark → N_{eig}^4 contractions)
    - This also provides a volume averaging at the source (as well as the sink)

$$C_{ij}^{NN}(t,\mathbf{p_f},\mathbf{q_f},\mathbf{p_i},\mathbf{q_i}) = \sum_{\mathbf{x_f},\mathbf{y_f}}\sum_{\mathbf{x_i},\mathbf{y_y}} e^{i(\mathbf{p_f}\cdot\mathbf{x_f}+\mathbf{q_f}\cdot\mathbf{y_f})} e^{-i(\mathbf{p_i}\cdot\mathbf{x_i}+\mathbf{q_i}\cdot\mathbf{y_i})} \langle 0|NN_i(t,\mathbf{x_f},\mathbf{y_f})NN_j^\dagger(0,\mathbf{x_i},\mathbf{y_i})|0\rangle$$

  - We used a stochastic variant which holds N_{eig} fixed as the volume varies [arXiv:1104.3870]
  - The correlation functions are now positive-definite $A_{ii} = \langle 0|NN_i|n\rangle\langle n|NN_i^\dagger|0\rangle \geq 0$
  - GEVP provides linear combo to project onto eigen-states

$$\langle NN(q)| \sim \sum_{\mathbf{p}}\sum_{\mathbf{x},\mathbf{y}} c(\mathbf{p}) e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \langle\Omega|N(\mathbf{x})N(\mathbf{y})$$

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- In order to take advantage of the positive-definite nature of the NN correlation function, we use the following fit function (implicit sum over l, q, p)

$$R(t) = \frac{r_0^2 e^{-\Delta E_0^{NN} t}\left(1 + r_l^2 e^{-\Delta E_{l,0}^{NN} t}\right)}{\left(1 + z_{q,n}^2 e^{-\Delta E_{n,0}^{q} t}\right)\left(1 + z_{p,m}^2 e^{-\Delta E_{m,0}^{p} t}\right)}$$

  - $r_l \sim O(1) \geq 0$
  - $z_{q,n} \sim O(1) \geq 0$
  - We include the same number of inelastic excited states in NN as in N, and then study the ground state vs the number of additional elastic excited states included in the analysis
  - We optimized the analysis to use the same values of t_{min} for all channels (irreps) rather than optimizing each one separately after finding a choice of t_{min} and n_{el} that is acceptable for all irreps